



Vlaams Supercomputer Centrum

Annual report 2015

www.vscenrum.be

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Preface

In 2015, the VSC, the Flemish supercomputer centre, - a partnership between the Flemish universities and the Hercules Foundation - came up to full speed.

The Flemish universities continued to expand their Tier-2 capacity. The VSC ensures that the researchers can migrate their applications easily between these machines so that the most suitable computer is used at all times.

To increase the visibility of the VSC, the VSC website was thoroughly upgraded, with the information now being provided on a targeted basis to academics and the industry. The number of training courses on the use of the Tier-1 and the Tier-2 organised for researchers from Flemish universities, strategic and public research centres, but also companies, was stepped up. All relevant information is also widely disseminated via VSC Echo, the electronic newsletter of VSC.

For the allocation of computing time on the Tier-1, the Board of Directors approved a slightly modified regulation, whereby a panel of international experts was again appointed for the evaluation of the applications. In 2015, applications were assessed on three occasions. A total of 109,704 node days were allocated to 32 projects. Researchers are charged a small portion of the costs to make everyone aware of the significant investments made by the Flemish government in the HPC infrastructure. Costs are also charged for the use of scratch disk space, with 1 TB being provided free of charge per application.

The User Committee maps the users' needs and organised a successful User Day at the end of 2015.

Special attention was also paid to collaboration with companies. With the help of the Industrial Board, initiatives were developed to highlight the advantages of a collaboration with the VSC: professional support, customised training as required, but above all embedding within an academic environment. The first Industry Day in early 2015, not surprisingly, attracted a large crowd.

2016 is set to be a challenging year for VSC, as it is the year in which the structural reforms announced in the policy note of minister Philippe Muyters, will take shape. Not only will the activities of the Hercules Foundation be taken over by the FWO, Research Fund Flanders - a process in which continuity will be a top priority - but we are also eagerly awaiting the entry into service of the new supercomputer at KU Leuven which will be operational from mid-2016. We are looking forward to it!

KU Leuven: Jan Ooghe, Leen Van Rentergem
University of Antwerp: Annie Cuyt, Stefan Becuwe
Ghent University: Ewald Pauwels
University of Hasselt: Geert Jan Bex
VUB: Rosette Vandenbroucke
Hercules Foundation: Bart De Moor, Marc Luwel

About VSC

A short overview of HPC in Flanders

In the past half century, research and technological innovation have ensured that the information and communication technologies (ICT) developed extremely rapidly. Furthermore, ICT has also had, partly through the development of powerful computers, a considerable impact on research and innovation. High processing capacity (HPC) makes it possible to distil valuable information from ever larger volumes of data and to perform large computing tasks within feasible time frames.

In addition to theoretical work and experiments, HPC has opened up a third way of undertaking research: simulating reality in silicon. Large numeric simulations are not only used in fundamental research; they are also having a growing impact on the innovative capacity of a company, a sector or a country, because they are at the basis of the development of new products and services or the improvement of existing products and services. There are many examples: from more accurate weather forecasts and personalised drugs to safer, cheaper cars and attractive animation films.

At the start of this century, Flanders lagged behind in HPC. The universities had invested in local processing capacity and the government had allocated punctual funding, but an overall vision was lacking. In 2007, the Royal Flemish Academy of Belgium for Science and the Arts (KVAB) pointed out, in the report 'Memorandum of the KVAB about High Performance Computing (HPC) in Flanders', the growing importance of HPC and the need for Flanders to quickly take an initiative towards bringing it in line with the international developments.

In the European model for HPC, a distinction is made between three levels: the processing capacity which research institutes have at their disposal (Tier-2), the processing capacity which goes beyond the needs and costs of an individual institution and which is provided at regional or country level (Tier-1), and the super powerful processing infrastructure (Tier-0).

The KVAB report recommends installing a Tier-1 supercomputer in Flanders which must be accessible to universities, public research centres, and companies. It is emphasised that investing in a Tier-1 is only sensible if, at the same time, each university can be assured of its own Tier-2 capacity. It further points out that hardware and software on their own are not sufficient.

It is at least equally important to ensure there are sufficient competent employees who can train and support the researchers. High processing capacity is after all used by researchers from the most diverse disciplines. These are people who are familiar with their professional discipline but not necessarily with the advanced techniques that are necessary to make optimal use of software on supercomputers. Finally, the report also points to the international developments and possibilities that applications on Tier-0 machines offer to Flemish researchers.

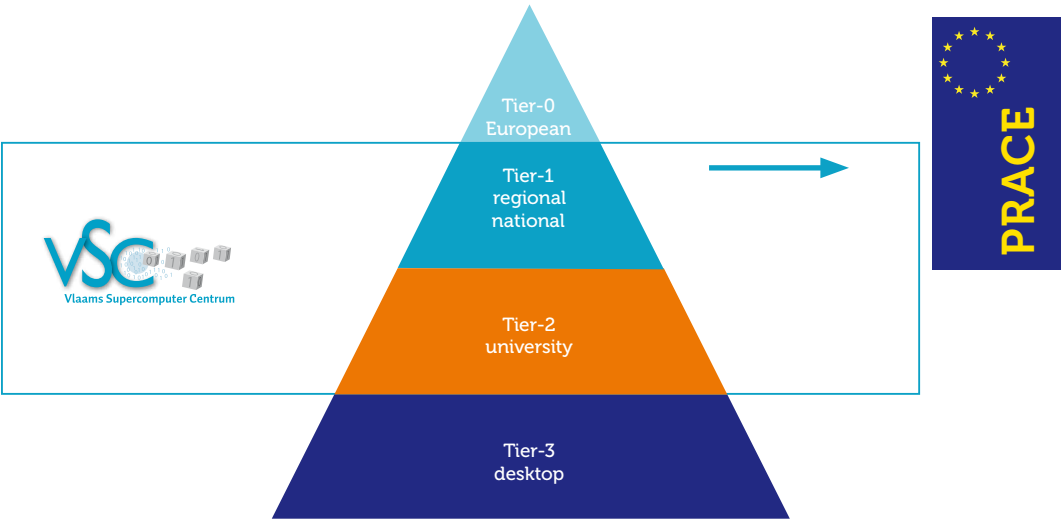
Almost simultaneously with this advice, the Strategic Forum for Research Infrastructure (ESFRI) decided to consider the proposal for Partnership for Advanced Computing in Europe (PRACE) of strategic importance for the European Union and to include it in the ESFRI roadmap.

In the following years, the recommendations of the KVAB were largely achieved. In 2006, the Flemish Minister responsible for Science and Innovation granted the Flemish Supercomputer Centre (VSC), a consortium of all Flemish universities, project-based funding in order to upgrade and expand the Tier-2 capacity for these institutions. Resources were also freed up for the salaries of employees who support the users and for implementing a study about the installation of a Tier-1 supercomputer in Flanders.

As part of the first call for large scale research infrastructure published by the recently founded Hercules Foundation in 2007, the VSC submitted an application for additional funding for the Tier-2 infrastructure. The Hercules Science Committee that advises the Board of Directors of the Foundation on the scientific quality of applications, judged this file positively, but advised the responsible Flemish minister to provide the necessary resources for the installa-

1 ESFRI: for details, go to http://ec.europa.eu/research/infrastructures/index_en.cfm?pg=esfri





tion of a Tier-1. Based on this, the Government of Flanders allocated a one-off funding for the purchase of a Tier-1 supercomputer.

Ghent University was prepared to provide the accommodation from its own resources. At the end of 2012, the Tier-1 supercomputer was officially taken into use. This took place with the resources that were allocated in 2008 and supplemented with part of the funding from the Hercules Foundation. This was used to fund employees at every university for the training and support of users. As supplement to the government subsidies, these institutions use their own resources to fund an important part of the costs and additional staff. The universities do consider the expansion of large computing capacity of strategic importance.

Sustaining and further expansion of a performing HPC infrastructure based on project-based funding reached its limits at the end of 2011. In 2012, the Government of Flanders allocated €1.5 million of structural funding to the Hercules Foundation for subsidising HPC at research centres. From 2013, this was raised to €4 million.

Supercomputer infrastructure has, however, a limited lifetime. The maintenance contract for the first Tier-1 supercomputer at Ghent University will expire at the end of 2016. However, continuity is ensured, as the second Tier-1 in Flanders, housed at KU Leuven, will become operational from the end of 2016.

The Flemish model

For the expansion of HPC in Flanders, the consortium model offers important benefits and furthermore reduces the costs. The Tier-1 and the Tier-2 computers are connected together via BELNET, the federal research network, and applications can migrate to the machine that is best suited to them. The employees are appointed to the five Flemish universities but form an integrated team that is responsible for the training and the support of users. For specialised support, each institution can make use of the specialist, irrespective of where he or she is employed. As already indicated, the universities invest with their own resources in the HPC infrastructure and they can make use of the central services of these institutions. Furthermore, the embedding in an academic environment offers opportunities for the collaboration with industrial partners.

The lack of structural funding appeared not to be the only obstacle in the further expansion of HPC in Flanders. There was also a need for a more structured framework for consultation between the universities and for a greater involvement from the strategic research centres and the other Flemish public research centres. There was a need for a clear, designated point of contact for the government and for additional initiatives to inform companies about the possibilities of HPC and to support these so that they can make efficient use of them.

At the proposal of the Flemish minister responsible, the Flemish Parliament approved a regulatory framework for this. The Flemish Parliament Act of 5 July 2013 concerning a structural regulation for large processing capacity for research and innovation and concerning the coordination of the legislation pertaining to scientific and innovation policy (HPC act) retains the benefits of the university consortium but lays the basis for improving its operation.

The assignment for the Hercules Foundation was widened with the structural funding of HPC and the management of the Tier-1. In implementation of these legislative provisions, the Board of Directors approved an amendment to the articles of association of the Hercules Foundation. In order to increase the role of the strategic research centres, the composition of the Board of Directors of the Hercules

Foundation, the mandate of which lapsed at the start of 2014, was changed.

After the adoption of this act, the Board of Directors of the Hercules Foundation decided to strengthen the role of the work group that consists of the staff of the Foundation and the persons who are responsible at each university for the coordination of the HPC activities. **The VSC Steering Group** meets monthly. During these meetings, operational agreements are made and also strategic advice is given to the Board of Directors.

In order to increase the collaboration with the companies but also with the non-profit sector, the act provides for the creation of an **Industrial Board** whose chairman is from the business community and who is also a member of the Board of Directors of the Foundation.

This board assists in devising a policy to increase the involvement of Flemish industry in High Performance Computing and to stimulate collaboration with the VSC, as well as to effectively promote the use of supercomputing in the development of innovative products and services.

The following members of the advisory board were appointed by the Flemish Government on 21 February 2014: Mia Vanstraelen (chairwoman), Herman Van der Auweraer, Ludo Lauwers, Christian Van de Sande, Saskia Van Uffelen, Charles Hirsch. In various brainstorm sessions with the HPC coordinators, shape and direction were given to a VSC policy that is directed more and better at Flemish companies and SMEs. The concrete presentation of what is available at the VSC and the organisation of the VSC Industry Day at Technopolis on 27 January 2015 were direct results of this.

For the purpose of providing advice on user needs and formulating proposals to improve the service, including user training, the Board of Directors of the Hercules Foundation installs a **User Committee** of at least seventeen members, on the recommendation of the associated universities and colleges, the strategic research centres and the Industrial Board. One member is appointed by the Flemish minister responsible for science and innovation. In addition, each university has its own user committee.



The members were appointed for a term of three calendar years starting on 26 June 2014.

Members User Committee 2015

| nominated by | name | institution |
|---------------------|--------------------------|-----------------------|
| Flemish Government | Francisco Hernandez | VLIZ |
| Association Leuven | Dirk Roose | KU Leuven |
| | Nicole van Lipzig | KU Leuven |
| | Nele Moelans | KU Leuven |
| Association Ghent | Veronique Van Speybroeck | Ghent University |
| | Dirk Van den Poel | Ghent University |
| | Veronique Hoste | Ghent University |
| Association Antwerp | Michele Giugliano | University of Antwerp |
| | Wouter Herrebout | University of Antwerp |
| Association Brussel | Frank De Proft | VUB |
| Association Limburg | Niel Hens | University of Hasselt |
| SOC | Clemens Mensink | VITO |
| | Steven Maere | VIB |
| | Piet Demeester | iMinds |
| | Wilfried Verachtert | IMEC |

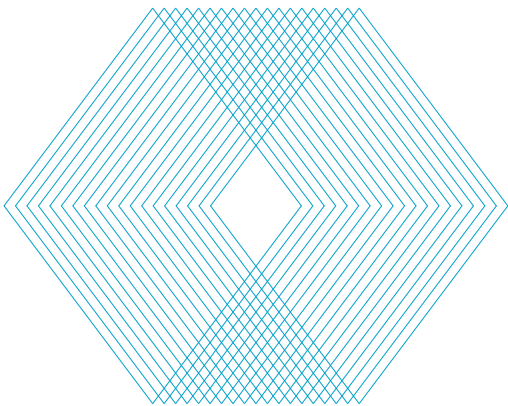
To keep in touch with the needs of new users, it is desirable that a number of members can be replaced at periodic intervals.

In 2015, the User Committee provided advice on the regulation applicable to the Tier-1 and organised a successful User Day on 30 November 2015.

Funding of Tier-1 and Tier-2

In 2012, the Flemish Government allocated a one-off allowance of €5 million for the upgrading and expansion of the Tier-2 infrastructure. From 2012 the Hercules Foundation has had access to structural funding for HPC. In 2013, 2014 and 2015, €4 million was available for this. These resources were used for funding of:

- staff costs for the operation of the Tier-1 (€190,000);
- staff costs for training and support of users of both Tier-1 and Tier-2 (€1,425,000); (For this amount, the five Flemish universities can subsidise in total the equivalent of 15 FTE.)
- part of the energy costs of the Tier-1 (€175,000);
- investment and operating costs for the Tier-2 infrastructure (€2,210,000); (The universities have mainly used this last amount for supplementary investments in Tier-2. These institutions finance the energy and operating costs of the Tier-2 from their own resources.)



In the table below, a summary is given of the distribution of this amount of €4 million over the five Flemish universities.

| Heading | Tier-1 | KU Leuven | University of Hasselt | Ghent University | VUB | University of Antwerp | Total |
|-------------------|-----------|-------------|-----------------------|------------------|-----------|-----------------------|-------------|
| Staff in FTEs | 2.0 | 5.0 | 1.0 | 4.0 | 2.0 | 3.0 | 17 |
| Staff in € | € 190,000 | € 475,000 | € 95,000 | € 380,000 | € 190,000 | € 285,000 | € 1,615,000 |
| Operation Tier-1 | € 175,000 | | | | | | € 175,000 |
| Hercules key 2013 | | 0.4354 | 0.0300 | 0.3190 | 0.1004 | 0.1152 | 1.0000 |
| Operation Tier-2 | | € 962,234 | € 66,300 | € 704,990 | € 221,884 | € 254,592 | € 2,210,000 |
| Total | € 365,000 | € 1,437,234 | € 161,300 | € 1,084,990 | € 411,884 | € 539,592 | € 4,000,000 |

For the allocation of the subsidies, the Hercules Foundation concluded an agreement with each university in which it was agreed that the spending of the allocated resources can be spread over two budgetary years. The allocated resources must be justified with receipts and a spending report must be submitted about the use to which the funding has been put, which should include information about the use of the Tier-1 and Tier-2 infrastructure.

Strategic plan for large computing power for research and innovation in Flanders – 2015-2020

In the run-up to the elections for the Flemish Parliament of May 2014, the Board of Directors of the Hercules Foundation drew up a strategic plan for large computing power for research and innovation in Flanders, for the period 2015-2020. This plan is updated annually to consolidate and further expand the outlined path.

This approach is based on the following findings:

- Developments within the ICT sector are taking place so rapidly that resources are necessary every 2 to 3 years for both Tier-1 and Tier-2 in order to update or expand the infrastructure;
- Investments in hardware and software are only meaningful if they are used efficiently. For this highly qualified staff are necessary to train and support the researchers;
- A limited but trained staff is required to inform the Flemish companies and also the non-profit organisations about the possibilities that HPC offers for improving their competitive position and for supporting them and for making use of all these possibilities;
- Flanders should further link itself to the international HPC community. In the first place in PRACE so that the possibilities offered can be better used (e.g. monitoring technological developments, models for collaboration with companies, training etc.).

In order to address these challenges, additional funding is necessary for both Tier-1 and Tier-2. But an increase in VSC staff is also necessary to satisfy the growing demand for training and support in a high qualitative way. The amount of €4 million at the disposal of the Hercules Foundation in 2015 must be raised to €10 million per year. Investment in new hardware will be spread over two budget years 2015 and 2016. In comparison with foreign HPC centres, this is still a modest funding.

The second Flemish Tier-1

The first Flemish Tier-1 supercomputer, installed at Ghent University, was taken into service in the first half of 2013 and needs replacing. On 20 July 2012, the Flemish Government stipulated the working method for the selection of the university that would be responsible for the accommodation of the second Tier-1. The Board of Directors of the Hercules Foundation decided on 21 October 2014 to conclude an agreement with the KU Leuven for the purchase and the accommodation of the second Flemish Tier-1.

With an amendment of the budget for 2015 of the Hercules Foundation, the Board of Directors decided to earmark an amount of €5.5 million from the investment allowance for the purchase and installation of the second Tier-1: €1,950,000 in 2015 and €3,550,000 in 2016. The latter on condition that the Flemish Expenditure Budget 2016 was approved. A not unimportant fact is that KU Leuven has made available a fully equipped room for the accommodation of this machine.

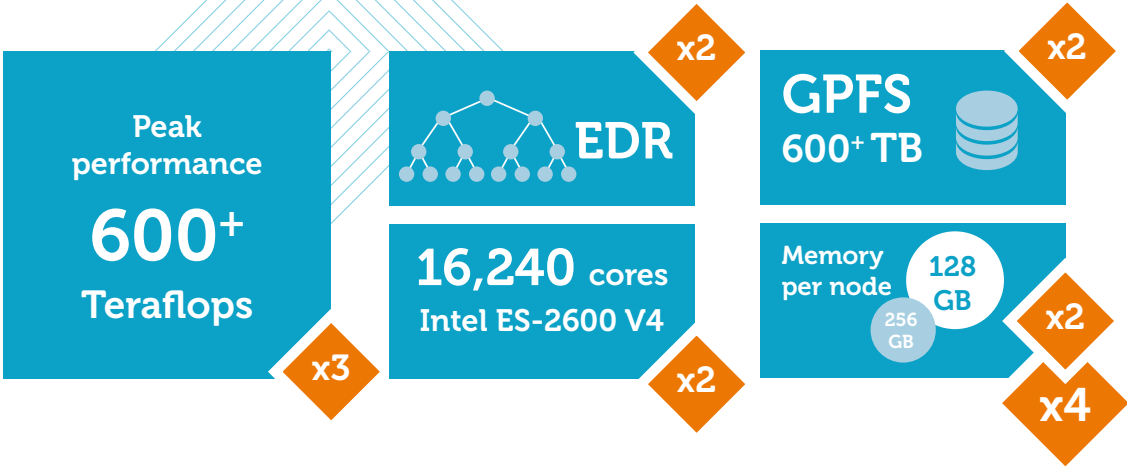
The new Tier-1 supercomputer therefore represents an investment of €5.5 million. The company NEC was selected to build the machine through a public tender procedure.

The supercomputer will have a theoretical peak performance of more than 600 TFlop/s. This makes it three times as fast as the first Flemish supercomputer, which is housed at Ghent University and already 3 years old. The supercomputer will be equipped with the latest Intel processors. The memory, internal network, and storage capacity, too, will be adapted to the complex problems that the computer will have to solve. The new machine will be installed at KU Leuven in the middle of 2016. It will be one of the 200 fastest computers in the world.

The new Tier-1 supercomputer will support research into, for instance, renewable sources of energy or the development of new materials and medication. The computer will also enable researchers, for instance, to create even more detailed climate models or to map the climate on other planets. For fundamental research, too, the new Tier-1 opens up new possibilities.

Flemish minister Philippe Muyters: *“The Flemish Government is committed to investing in research and innovation. Our research institutions are among the best in the world. We can only maintain and strengthen that top position if we keep investing. The supercomputer can play a crucial role in a wide range of fields. It fills me with pride to see that the Flemish Government has fully played its role in bringing this about.”*

From Tier-1 to Tier-1b



Tier-2 infrastructure and projects per organisation

Operation and use

In this section we provide an overview of the Tier-2 infrastructure available within the various Flemish universities. We also illustrate its use.

KU Leuven and University of Hasselt

For the Tier-2 infrastructure, KU Leuven and the University of Hasselt work together.

The infrastructure consists of:

- 2 clusters / 7 partitions
- 150 TF
- 5312 CPU / 71808 accelerator cores
- 32 TB memory

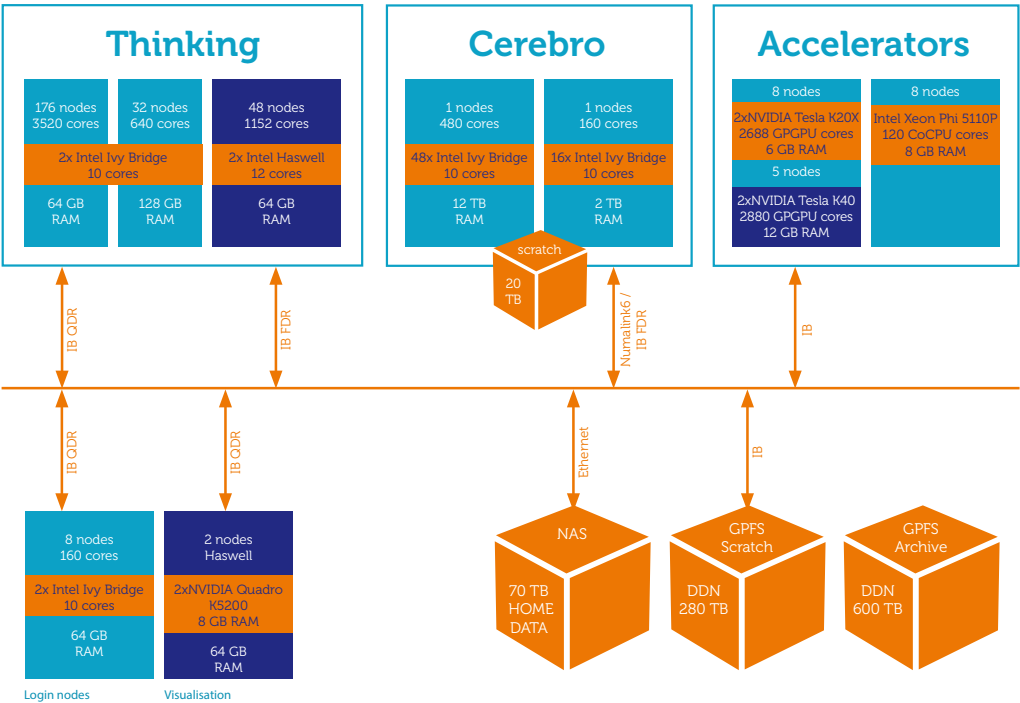


Figure 1 - KU Leuven Tier-2 infrastructure

The thin node cluster *ThinkIng*, was delivered at the end of December 2013 by HP. The system went into production on 15 July 2014. In March 2015, 48 nodes were added, with a new generation of processors (Haswell). This brought the number of nodes to 256 and total system capacity to 138 TFlops.

In 2015, the accelerator section was expanded with 5 nodes. These new nodes contain 2 latest generation GPU cards (NVIDIA K40). The accelerator section is still a more experimental environment. It does not have the capacity to perform large-scale computations. The expectation is that more application software, specific libraries or implementations of new algorithms will become available that use GPU acceleration. The accelerator section gives researchers the opportunity to evaluate these things.

In 2015, 2 specific visualisation nodes were added to the cluster. The GPUs (NVIDIA Quadro K5200) in these nodes are used for visualisations, not for general purpose computing.

Ghent University

Ghent University has been investing for several years in the development of a powerful Tier-2 infrastructure. Today it consists of:

- 5 clusters
- 174 TF
- 8768 CPU cores
- 49 TB memory

The Tier-2 infrastructure is built up of various clusters, serving specific characteristics. In the course of 2015, the four oldest clusters were taken out of service: batch clusters *haunter* and *gastly*, MPI cluster *gulpin* and cluster *dugtrio*. Their replacement was started proactively in 2014 with the purchase of clusters *golett* and *phanpy*. Both went into production in June 2015.

At end of 2015, *swalot* was purchased (Dell), a new MPI cluster to facilitate multi-node jobs. This cluster will be put into production by June 2016.

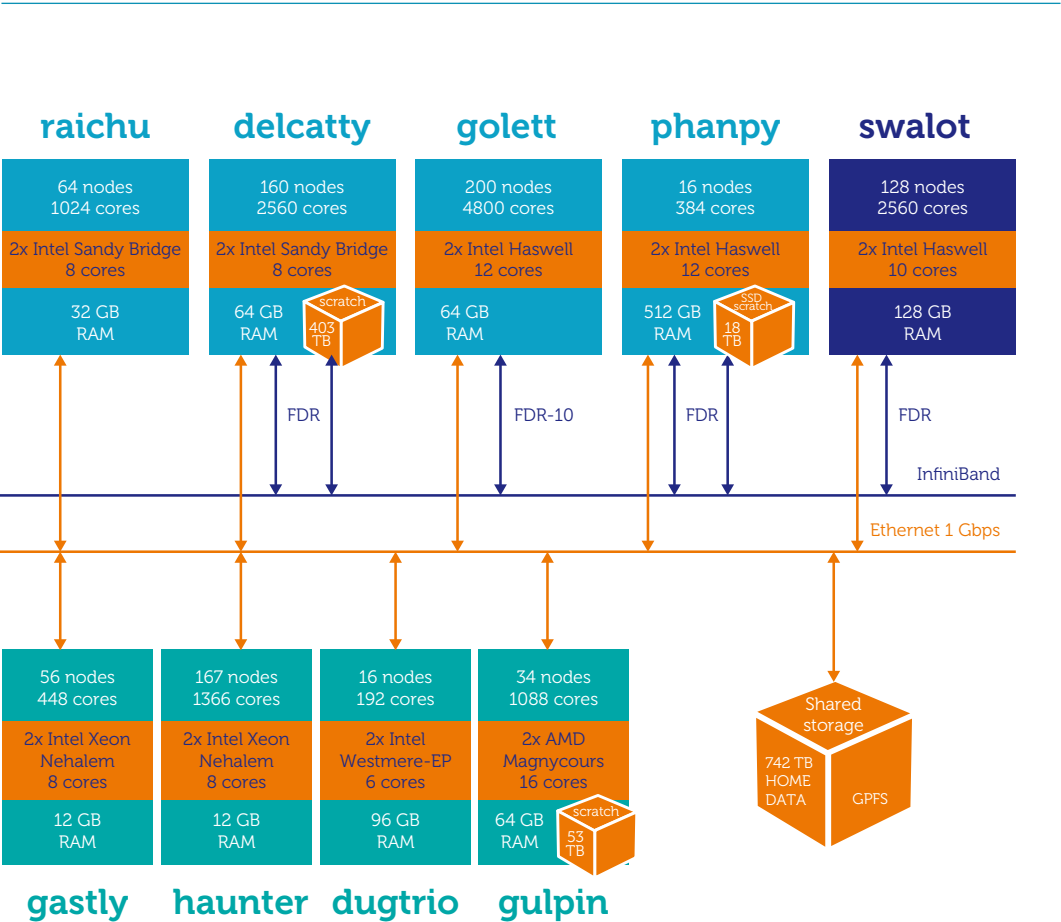


Figure 2- Ghent University Tier-2 infrastructure

University of Antwerp

For the University of Antwerp, large processing capacity for research is a strategic priority. The Tier-2 infrastructure consists of:

- 2 clusters / 4 partitions
- 90 TF
- 4992 CPU cores
- 12 TB memory

In the course of 2014, the *Hopper* cluster was supplied by HP to the University of Antwerp. Initially the cluster consisted of 120 nodes. Of these, 24 are so-called *fat nodes*, met 256 GB memory. This allows researchers with larger memory demands to make more efficient use of the cluster.

In the autumn, 48 nodes were added. Thus, at the end of 2014, the University of Antwerp had a cluster with a theoretical processing power that is five times larger than Turing, the previous cluster that is still in use. Together with *Hopper*, a new storage system was also taken into use.

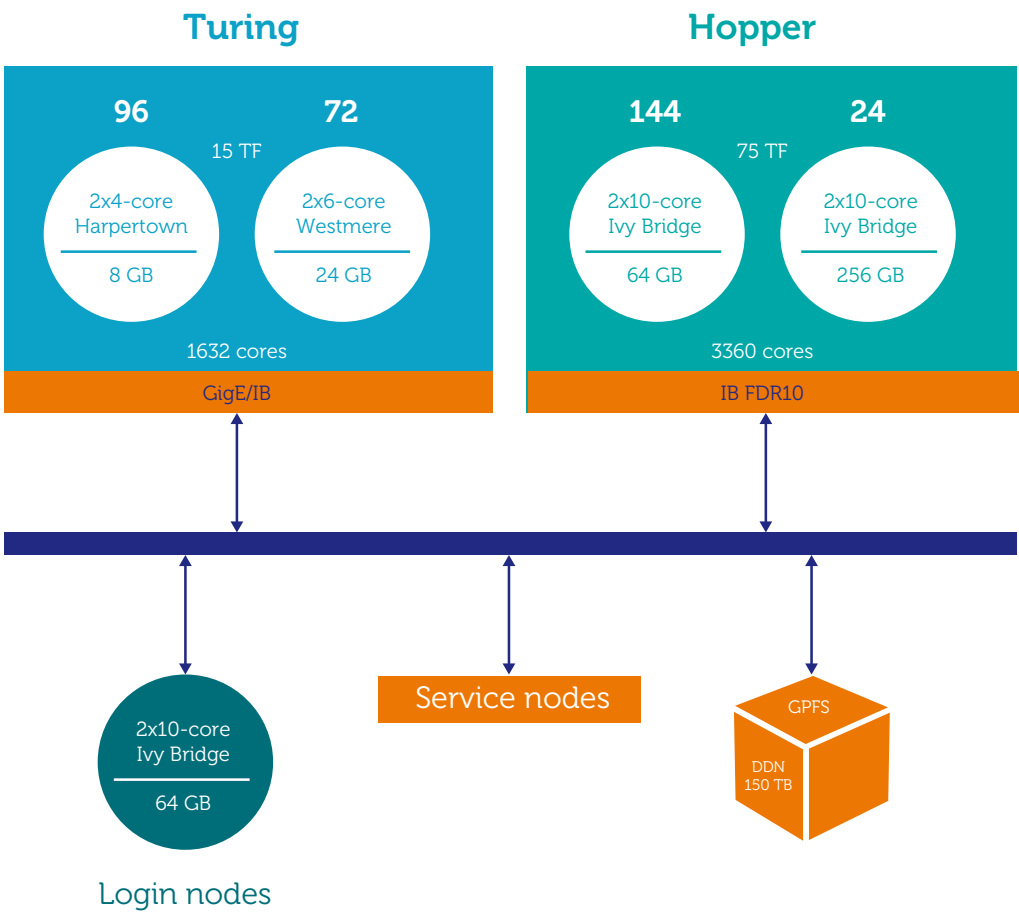


Figure 3 - University of Antwerp Tier-2 infrastructure

Vrije Universiteit Brussel

The Tier-2 environment at the VUB looks as follows:

- 1 cluster / 5 partitions
- 16 TF
- 2436 CPU cores / 32496 accelerator cores
- 14 TB memory

The VUB has chosen to systematically expand its infrastructure within the same Hydra environment. The result is a highly heterogeneous cluster that meets the needs of the various research groups. In 2015, a number of the oldest partitions (Shanghai) were taken out of service. 292 TB of storage space was added.

In addition to its own Tier-2 infrastructure, the VUB - together with the ULB - manages the grid infrastructure, which is used, among other things, for processing data that are collected during experiments with the Large Hadron Collider (HPC) at the CERN. The 1.2 PB extra storage capacity was put into service in 2015, bringing the total available storage capacity to 2.3 PB. A number of old nodes were taken out of service. Expansion of the processing capacity is planned for 2016.

Finally, the VUB has its own test configuration for the cloud infrastructure.

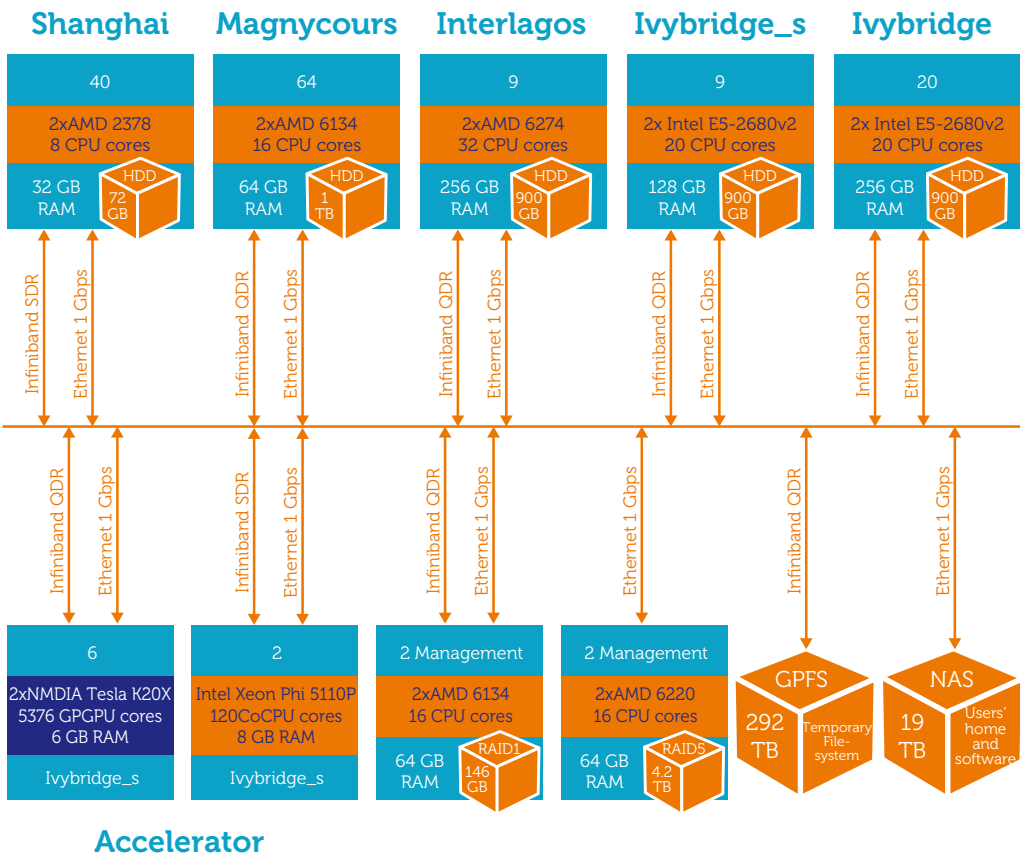


Figure 4 - VUB Tier-2 infrastructure

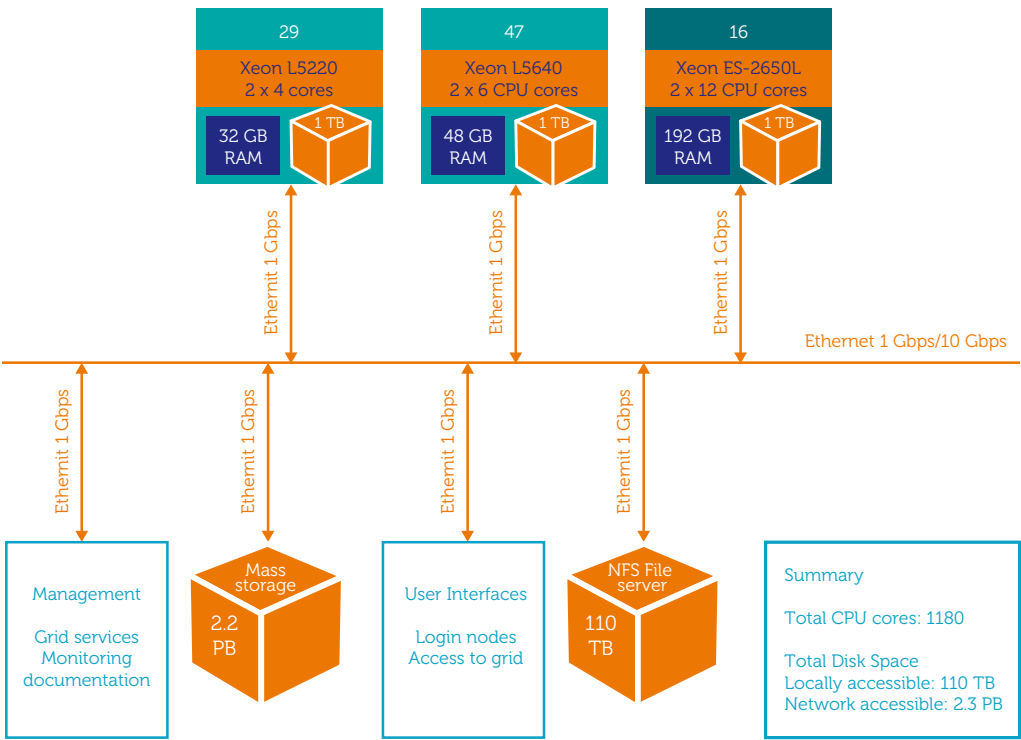


Figure 5 - VUB grid infrastructure

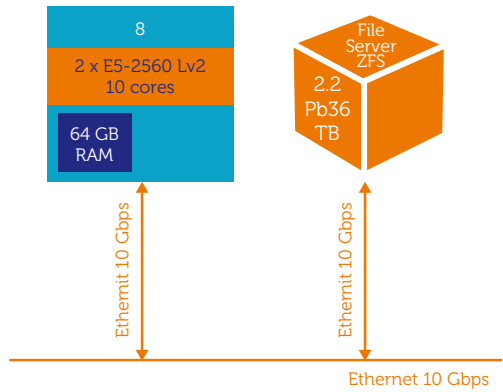


Figure 6 - VUB cloud infrastructure

Use

Having described the infrastructure, we now present an overview of the use of the Tier-1 and the Tier-2.

For monitoring the use, the VSC has a central XDMoD infrastructure that collects all data from the various clusters and generates the necessary overviews.

CPU hours: Total by resources

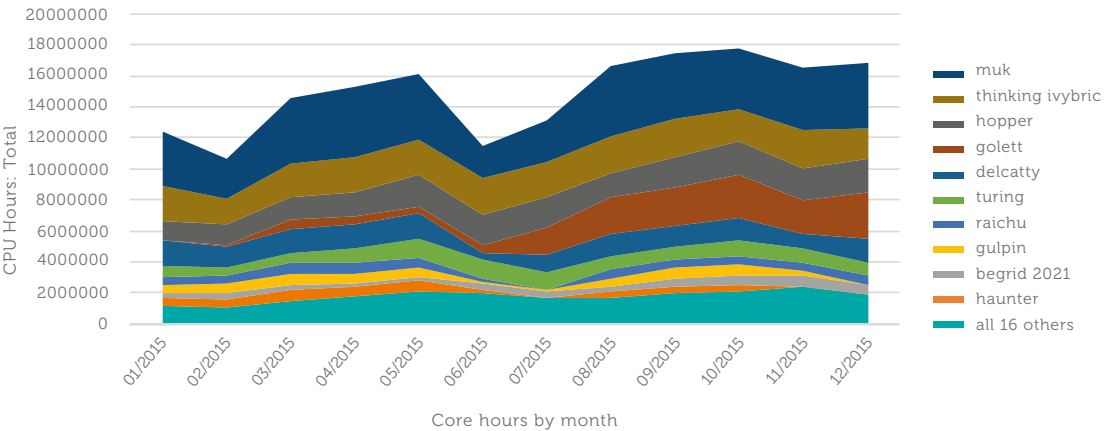
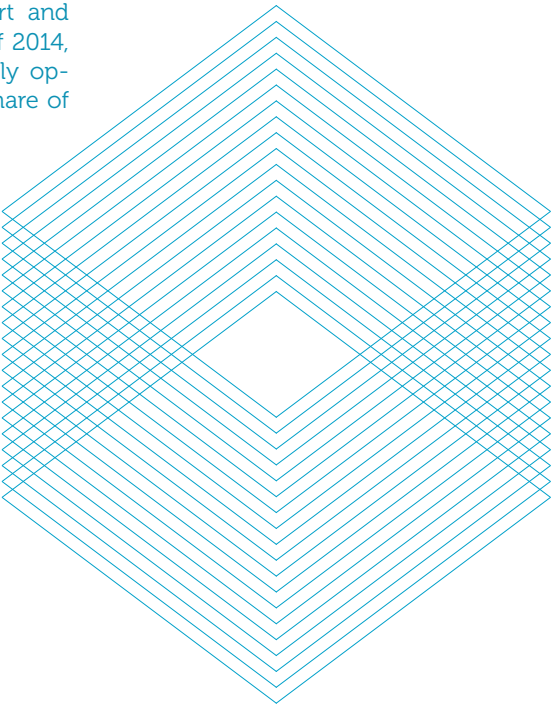


Figure 7 - Cumulative use of the Tier-1 and Tier-2 infrastructure

Figure 7 shows the cumulative use of the Tier-1 (muk) and Tier-2 infrastructure. There is a noticeable difference between the start and the end of the year. Towards the end of 2014, several new Tier-2 clusters became fully operational, thereby increasing the total share of Tier-2.



Used CPU hours on thin node clusters
KU Leuven

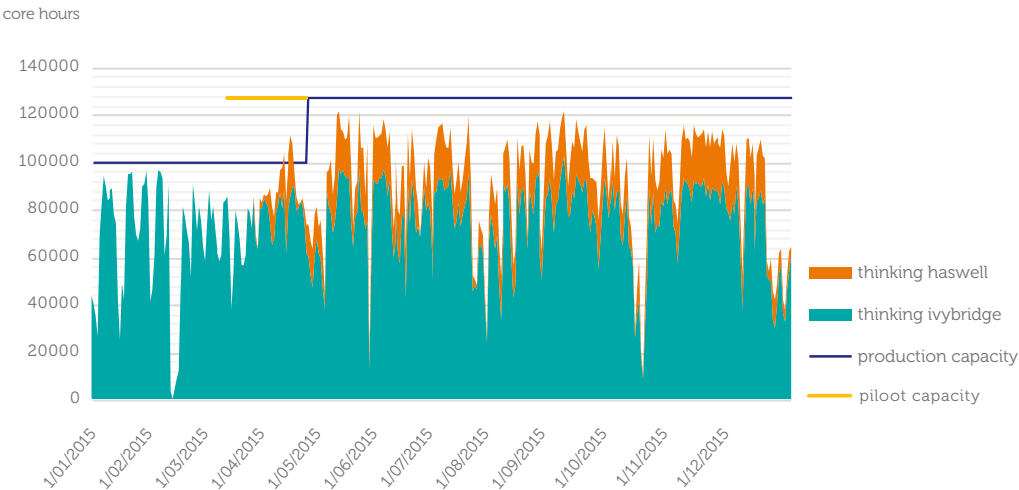


Figure 8 - Use of the KU Leuven infrastructure

Figure 8 gives an overview of the use of the KU Leuven infrastructure. The graph shows the cumulative use of the various thin node clusters at KU Leuven. The cluster consists of a partition with IvyBridge processors and a new, smaller, partition with Haswell processors. The IvyBridge partition regularly has an 80-90% utilisation rate during the day and also the Haswell partition showed good utilisation after the running-in period. In mid-October, the cluster required a prolonged downtime, which was used to reorganise the file system.

Used node hours on shared memory cluster
KU Leuven - University of Hasselt

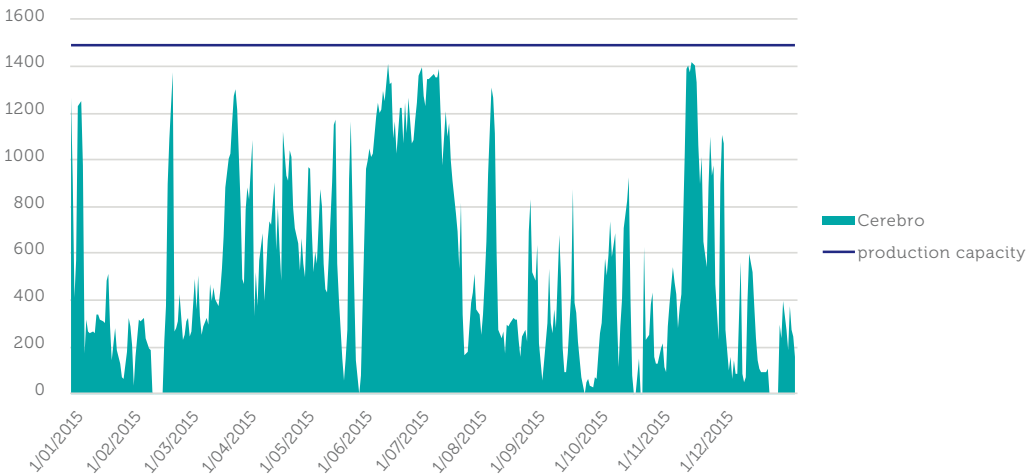


Figure 9 - Use of shared memory

Used node hours on GPU cluster
KU Leuven - University of Hasselt

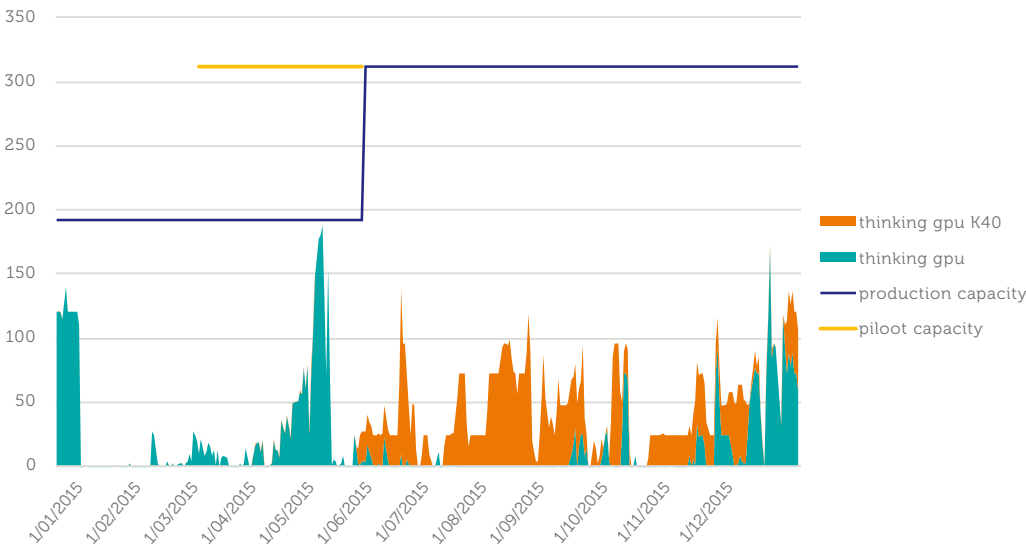


Figure 10 - Use of accelerators

In addition to the thin node processing cluster, KU Leuven also has a shared memory machine and a configuration with GPU and Xeon Phi accelerators. The use of these machines is expressed in node hours and not in core hours. This is because frequently the complete node is used because of the memory needed or because of the accelerators; and this without all CPU cores in the machine necessarily being used.

The shared memory machine is used less intensively than the thin node cluster, but also regularly shows good utilisation. Its large memory capacity makes it perfect for running jobs that are less or not suitable for the thin node cluster.

In 2015, GPU use was still limited. At the end of 2015, however, there was more interest for the GPUs, a trend that is continuing in early 2016. The Xeon Phi accelerators are not included in the graph. The fact that not much code has yet been developed for the Xeon Phi accelerators, is also apparent from the very low use. This might well change with the future generation of Intel processors.

Used CPU hours on thin node clusters
Ghent University

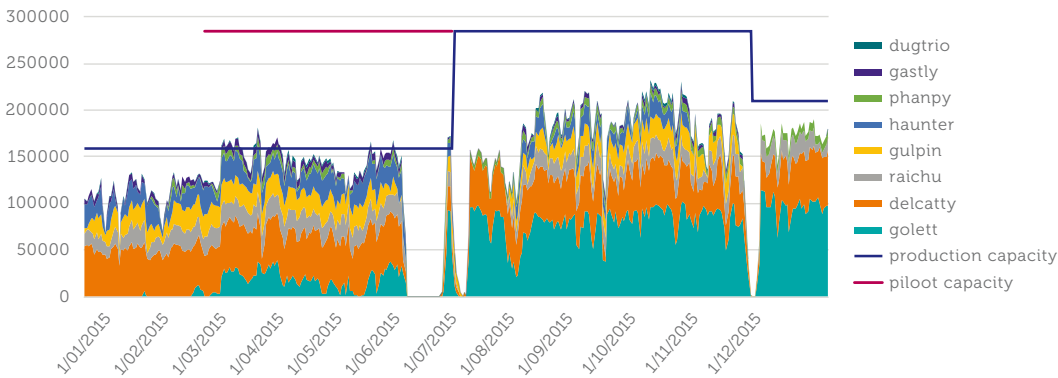


Figure 11 - Use of Ghent University infrastructure

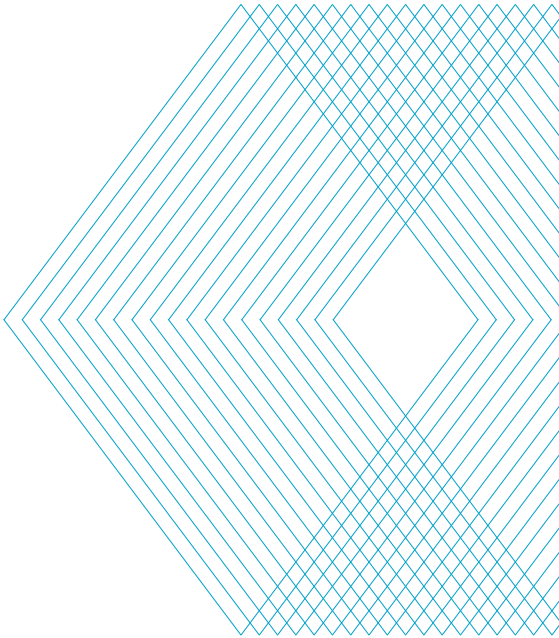
Figure 11 shows the cumulative use of all HPC clusters at Ghent University in 2015.

A second dip in capacity in November 2015 was due to a scheduled maintenance of a few days.

In the course of 2015, two new clusters (*golett* and *phanpy*) were taken into production. These were for some months run in parallel with the four older clusters they are replacing, which resulted in almost a doubling of the total capacity of the processing infrastructure at Ghent University. After the older clusters were removed from service, capacity stabilised at 130% of the level at the start of 2015, i.e. a 30% net increase in capacity.

On average, 75% of the total processing infrastructure at Ghent University is used. Two dips in usage are shown in the above figure.

Due to a severe hardware failure in the central HOME/DATA storage unit in early June 2015, all Tier-2 computer nodes could not be used for an extended period of time. The problem was solved as quickly as possible in consultation with the supplier. The hardware failure had corrupted part of the central storage data, which had to be restored from an emergency copy. This was a time-consuming process because of the size of the storage (737 TB). All clusters were released in phases in July 2015. Thanks to the efforts of our team, none of the users eventually suffered any data loss.



Used CPU hours on thin node clusters
University of Antwerp

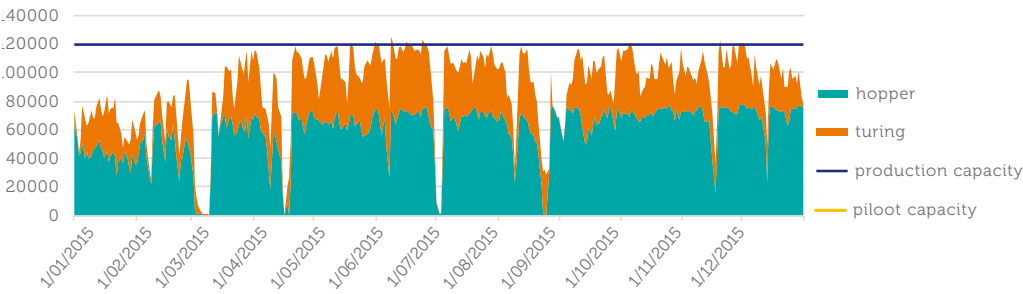


Figure 12 - Use of the University of Antwerp infrastructure

The graph of Figure 12 shows the cumulative use of the Turing and Hopper clusters at the University of Antwerp. A number of interruptions can be seen on the graph. Thus, works were carried out on the data centre infrastructure in March, April and August; there was a scheduled maintenance window at the end of June and start of July, and there were also a few short interruptions caused by power failures. Aside from these interruptions, the clusters are very well used. As a result of the reporting method (related to so-called hyper-threading), a utilisation of more than 100% is sometimes shown.

Used CPU hours on thin node clusters
VUB

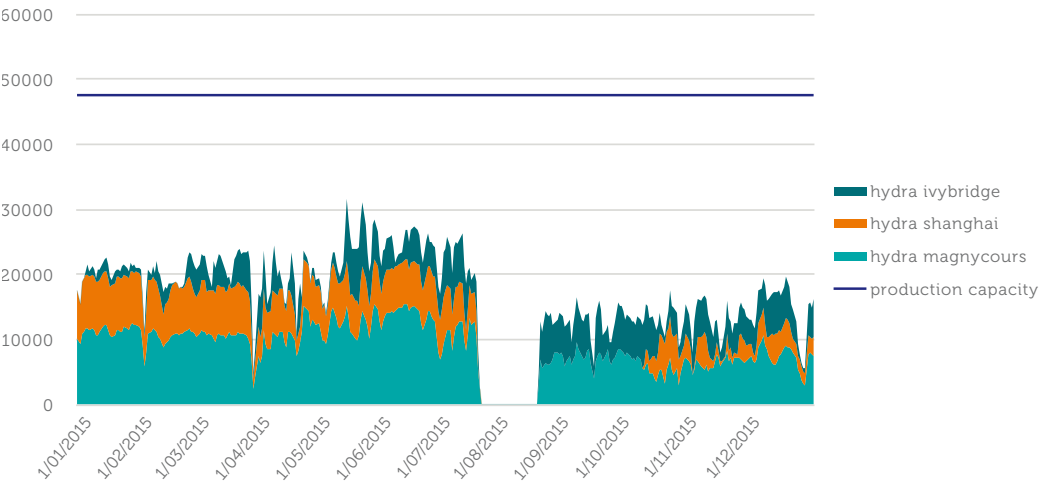


Figure 13 - Use of the VUB infrastructure

In the summer period, extensive maintenance was carried out on the VUB-ULB data centre. Major electricity works on the ULB campus and in the data centre required a period of a few weeks of complete downtime. Also during this period, firmware and operating system upgrades were carried out on the cluster and a new storage system was added. In August, the cluster became available again, but the job logging system was not yet operational, hence a longer period over which no figures can be reported.

After the start-up in September, the Shanghai nodes were no longer included in the reporting. As planned, they were taken out of production, but were subsequently put back into production for jobs that require much processing power.

After the start-up there was a decrease in use due to a bug in the new version of the scheduling software, which remains to be fixed by the supplier.

The Hydra clusters run both jobs that use all processing cores in a node and jobs that do not use all cores but require the complete node because of memory requirements. This mix leads to a distortion in the utilisation rate by core hours or node, which is why the graph does not indicate the total number of available core hours.

BEgrid 19, BEgrid 20-21 and BEgrid 22 are the three parts of the BEgrid cluster at the VUB. The BEgrid 22 nodes were taken into service in March 2015. The utilisation of the grid cluster is increasing and an expansion is planned for 2016.

**Used CPU hours on the BEgrid clusters
VUB**

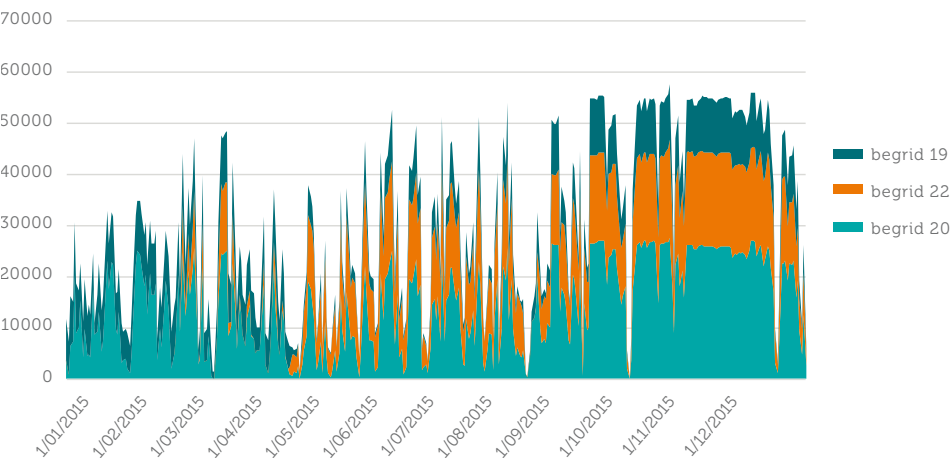


Figure 14 - Use of BEGrid cluster at VUB

Projects

The expansion of the large processing capacity for research is tackled within the VSC in a project-based way.

In this section, we present an overview of the projects worked on in 2015.

Account page

On the account page, new users must upload their public key and existing users can change their keys and other characteristics. The account page is also the central point for managing access to the Tier-1. This page therefore plays a key role in the VSC story. The account page is now fully operational. The interface was reworked, fields of science and storage quotas per user were added, and the migration from version 1.8 to the django framework was implemented.

Security logging and policies

In 2015, this project focused mainly on the Tier-1, as part of the discussions with an industrial user. Topics addressed included the following: security of the housing data centre, descriptive security policies, review and description of the system set-up and the network connectivity, and data encryption. The knowledge arising from this project will also be applied to the new Tier-1 machine.

Monitoring and reporting: XDMoD

Monitoring (the use of) the infrastructure is a key aspect of sound system management. It allows the identification of scheduling problems, sub-optimum use of machines, user needs, etc. This information is also important for future purchases of machines and software. After the test phase in 2014, XDMoD is now fully operational and all available data is processed. The environment is used to generate the use statistics included in this annual report. Activities planned for 2016 include the introduction of fields of science to enable more detailed reporting.

Website and marketing

The revised VSC website is up and running! Not only was the structure fully reworked, but also the content was updated. To keep the management as transparent as possible, the responsibility for the various website components was distributed among several employees.

Tier-1b

During the past year, the purchase of the second Flemish supercomputer was thoroughly prepared. The purchase procedure included, among other things, the selection of potential suppliers, the drafting of the specifications, and the final choice. The order was placed in the autumn of 2015.

Common user environment

In this project, common characteristics of the software environment are developed, implemented and documented for every machine that is accessible to VSC users. The results of this project are used every day by our users. It remains an ongoing project whose status is evaluated at regular intervals. All of this is also reflected in the available training material.

Training material

Various training programmes are organised within the VSC. The majority of these training programmes are open to all VSC users. The "Introduction to HPC" text is continuously maintained and updated. In addition to the specific course material, which, wherever possible, is listed on the VSC website under the description of the event, the user portal part on the website is also continually kept up to date and expanded.

Profiling and performance analysis

Having considerable processing power is useful, but efficient use of the available processing power is absolutely essential. The necessary tips and tricks are thus presented to the users in several seminars. In addition, users are taught techniques for optimising software codes. At the same time, users are familiarised with available tools.

User support

The user support can be divided into various components:

- answering questions from users (helpdesk);
- meetings with users / specific support;
- training and outreach.

The last item is discussed in the sections “Training” and “Outreach to Flemish companies”.

Answering questions from users

Here we look at the tickets that arrive at the helpdesk. There is no central VSC helpdesk. Each institution solves the questions and problems of its own users, both concerning their own Tier-2 infrastructure and the central Tier-1. If necessary, questions concerning Tier-1 are passed on to the helpdesk at Ghent University. For these questions, we distinguish 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 / University of Hasselt | Ghent University | University of Antwerp | VUB | Total |
|---------------|---|------------------|--------------------------|-------|-------|
| Tier-2 + grid | | | | | |
| accounts | 508 | 175 | 28 | 123 | 834 |
| software | 332 | 42 | 77 | 638 | 1,089 |
| others | 592 | 1,688 | 265 | 477 | 3,022 |
| | | | | | |
| Tier-1 | | | | | |
| accounts | | 17 | | | 17 |
| software | | 0 | | | 0 |
| others | | 154 | | | 154 |
| Total | 1,432 | 2,076 | 370 | 1,238 | 5,116 |

Meetings with users / specific support

On the one hand, we try to involve as many researchers as possible in the HPC story by examining whether and how they can make the switch from their desktop to the HPC infrastructure. On the other hand, we try to provide specific support to researchers.

Some examples:

- optimising existing work flows;
- optimising code;
- providing input to the writing of research projects;

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

KU Leuven and University of Hasselt

Daily support deals with questions regarding accounts, basic use of the cluster, and software installations. These questions come from users from groups who have been using the cluster for quite some time. Making the VCS infrastructure known to new research groups is an ongoing effort. However, also within groups that already use the cluster, specific actions may help to promote cluster use. In this way, more computational work can be performed more efficiently and in a shorter period as compared to a local infrastructure such as workstations and desktops.

New researchers are familiarised with the use of the cluster in regular introductory sessions or via a one-on-one consult where those already having some general prior knowledge of Linux and HPC receive sufficient information in just two hours in order to become productive on the cluster.

In 2015, specific actions and workshops were aimed at various groups. A group of researchers within the Department of Mechanics had long been using the local cluster, which in the meantime had become obsolete. A switch to the central VSC infrastructure was therefore indicated. A workshop was organised to facilitate the transition from the local to the central cluster.

The Animal Physiology and Neurobiology lab also took its first steps towards the cluster. This group works primarily with local workstations.

These researchers face a greater barrier as they first need to acquire a basic knowledge of Linux. The adaptation of the cluster use is slower and can only be successful if there is a "HPC champion" within the group.

Research conducted within the VIB requires much processing power. The focus was directed specifically at computations that require much storage capacity. The shared memory machine is best suited for this purpose. To introduce the users to the possibilities, the software stack was installed on Cerebro.

Flanders Hydraulics Research, a division of the department of Mobility and Public Works of the Flemish Government, needed more processing power to allow additional studies to be carried out. The processing capacity available in-house was inadequate. The FHR researchers received an info session on the use of the VSC cluster. Their software was installed and is now intensively used.

In 2015, we also participated in a number of courses that were organised by researchers, but that also use HPC. As part of the Bioinformatics Master's programme, 2 sessions dealt with HPC in general and use of HPC on VSC infrastructure in particular. This should lower the barrier for these young researchers to use HPC for their master thesis or in their future research career.

The Department of Computer Sciences organised a course "Coping with Big Data", which was also open to non-university researchers. For the exercises and examples, the HPC cluster was used.

The Department of Quantum Mechanics organised an "Intensive course on computational and theoretical chemistry for Erasmus Mundus Masters". In this course, the HPC staff gave an introduction to the use of HPC for quantum chemists.

To bring VSC to the attention of a wider group of people, VSC is also presented at events such as the Aviation Day - "Workshop facilitating the contacts between KU Leuven and aviation industry in Flanders" and the symposium for students Ea-Ict on Technology Campus De Nayer.

The basic support for researchers working at the University of Hasselt is provided via the

HPC helpdesk of the KU Leuven as this is the infrastructure used by the researchers.

More specialised support is provided on a one-to-one basis by Geert Jan Bex. The CenStat, Center of Molecular and Materials Modelling, Center of Environmental Science, Institute of Mobility, Management Information Systems and Theoretical Physics research groups all applied for this support in 2015. Here, it should be noted that a number of research groups took an active interest in the HPC infrastructure in 2015, which is a welcome trend.

Ghent University

In 2015, the HPC-UGent team organised introductory courses 'Introduction to HPC @ UGent' on demand for specific departments:

- Applied Materials Sciences (Faculty of Engineering and Architecture)
- Data Analysis (Faculty of Psychology and Educational Sciences)
- Applied Ecology and Environmental Biology (Faculty of Bioscience Engineering)
- Biochemistry and Microbiology (Faculty of Sciences)
- Sociology (Faculty of Political and Social Sciences)
- Research group Biofluid, Tissue and Solid Mechanics for Medical Applications (bioMMeda, Faculty of Engineering and Architecture)

In addition, more general user meetings attended by researchers from various research groups of Ghent University, were organised:

- Department of Architecture and Urban Planning (Faculty of Engineering and Architecture)
- Department of Information Technology (INTEC, Faculty of Engineering and Architecture)
- Department of Electrical Energy, Systems and Automation (Faculty of Engineering and Architecture)
- Department of Marketing (Faculty of Economics and Business Administration)
- Laboratory of Hydrology and Water Management (Faculty of Bioscience Engineering)
- Terrestrial Ecology Unit (TEREC, Faculty of Sciences)
- Department of Reproduction, Obstetrics and Herd Health (Faculty of Veterinary Medicine)

- Center for Molecular Modelling (Faculty of Sciences & Engineering and Architecture)
- Computational Biology research group (Faculty of Sciences Bioscience Engineering)
- Department of Medical Protein Research (Faculty of Sciences & VIB)
- Centre for X-ray Tomography (Faculty of Sciences & Bioscience Engineering)
- Data Mining and Modelling for Biomedicine (Dambi) research group (Faculty of Medicine and Health Sciences & VIB)
- BigN2N consortium (Bioinformatics Institute Ghent from nucleotides to networks)
- Evolutionary Systems Biology lab, department of Plant Systems Biology (Faculty of Sciences & VIB)
- Biomarked valorisation consortium Ghent University

However, user meetings were also organised for (potential) users from outside Ghent University:

- Bayer Cropsience
- J&J
- Siemens
- Umicore
- FEops NV (a spin-off of Ghent University)
- Bekaert NV

On 4 May 2015, the HPC-UGent team organised the workshop 'Big Data@UGent in practice' as part of the Big Data specialisation of Ghent University within the VSC. The general purpose of this workshop was to bring together all researchers within the network of Ghent University who are involved in Big Data projects, regardless of their scientific background. The specific objectives were to:

- establish a Big Data community at Ghent University, and beyond
- learn more about the subject, for experienced researchers as well as beginners
- offer a (first) opportunity to exchange experiences, discuss problems, showcase applications
- enable participants to perform a Big Data analysis on the VSC Tier-2 infrastructure in a hands-on session.

The scientific steering group of this workshop was broad-based, with several researchers from Ghent University and VIB, from the Faculties of Engineering and Architecture, Sciences, and Arts and Philosophy. The workshop was attended by over 200 researchers.

As a follow-up to this workshop, an edition of the annual BeNeLearn conference on Machine Learning and Big Data, will be organised for an inter-university and international audience in 2016.

University of Antwerp

On the one hand, we deal with questions from existing users and try to organise the computational work as optimally as possible, and on the other hand, we try to make the VSC known to other researchers to convince them of the potential benefits of using the central infrastructure. To this end, we target specific researchers/research groups. Each year we also organise two intro sessions.

In 2015 we put researchers from Pharmaceutical Sciences and Product Development on their way towards HPC. They are now frequent users of the infrastructure. Also other research groups from e.g. Biomedical Sciences, Bioscience Engineering and Chemistry have found their way.

Some examples of specific support:

- Optimisation of the work flow for the processing of short films that follow worms.
- Optimisation of the work flow for large batches of jobs that generated a tremendous amount of small files. Not only did this put a great burden on the file system (to the detriment of all users), but it also took up a large amount of valuable storage space.
- Implementation of checkpointing for long-term computations. This allows the infrastructure to be used more efficiently and computations to be restarted in case of problems as so to minimise loss of computing time.
- Support with applications for Tier-1 computing time.
- Support with (inter-university) project applications.

We discussed together with the VITO research group "Environmental Modelling" on the one hand, how computational expertise can be

deployed in VITO projects and, on the other hand, how VSC processing power can be used.

To disseminate information about the VSC also outside of the institution, we participated in the "UAntwerpen backstage" event on 17 March 2015. On a continuous knowledge market, companies were introduced to the available facilities of University of Antwerp (and the VSC) and thus given the opportunity to establish contacts.

In addition to training within the VSC, courses are also organised under the regular programme: "Scientific computing environments" and "(Parallel) programming".

The University of Antwerp has a user group which was formed in 2006 and meets twice a year. The user group consists of representatives from 12 groups and disciplines.

Vrije Universiteit Brussel (VUB)

In addition to the continued monitoring of existing users at Tier-2 and Tier-1 level, we assisted new potential Tier-1 users with the submission of a computing time proposal or a starting grant application.

We gave also special attention to researchers from the humanities who would also benefit from the use of more processing capacity than is available on their PC. These researchers usually do not have any experience with the use of Tier-2 systems. The best solution was to guide these people to the use of extra computing power in a cloud environment. In the meantime, a number of researchers from the department of psychology have embarked on this course.

The following courses are organised twice a year: "Introduction to Linux" and "Introduction to the use of HPC at the VUB".

The VUB has a HPC user committee, which meets approximately every two months and monitors the use and needs for HPC. The user committee consists of members from all faculties.

Staff

Since the infrastructure of the VSC (Tier-2 and Tier-1 infrastructure) is installed in the various university data centres, the staff are also employed at the various universities

Funding

On the one hand, each university needs staff for the operation of the Tier-2 infrastructure and the support of the end-users. For this, 15 FTE are subsidised. On the other hand, the institution where the Tier-1 supercomputer is housed has been allocated 2 FTE for its operation.

Since each university has its own employee policy and applies different remuneration principles, each FTE is paid a fixed amount of €95,000.

| Institution | number of subsidised FTE for Tier-2 operation and support |
|-----------------------|---|
| Ghent University | 4 |
| University of Antwerp | 3 |
| VUB | 2 |
| University of Hasselt | 1 |
| KU Leuven | 5 |
| Total | 15 |

| Institution | number of subsidised FTEs for Tier-1 operation |
|------------------|--|
| Ghent University | 2 |
| KU Leuven | 0.8 |

Effective staff deployment

Operating, maintaining and supporting the users of the various Tier-2 and Tier-1 configurations requires on the one hand more manpower than is provided for within the funding. On the other hand, a broad range of expertise is required that cannot be accumulated within one limited team. To address this, HPC technicians and support staff can make use of other experts who work in the ICT departments of the various universities. The universities deploy together 28 FTE for HPC operation and support. We should point out here that, because of an institution-wide regulation, the FTE who are deployed at the

University of Antwerp and are not paid by the Hercules Foundation, can only be included for a prescribed and maximum fraction of the deployment in this table.

| Institution | Number of VTE deployed for HPC | Number of heads involved with HPC operation and support |
|-----------------------|--------------------------------|---|
| Ghent University | 10.6 | 16 |
| University of Antwerp | 4.35 | 8 |
| VUB | 4 | 9 |
| University of Hasselt | 1 | 1 |
| KU Leuven | 8.25 | 16 |
| Totaal | 28.2 | 49 |

Profiles

In order to operate and support a HPC infrastructure effectively, various ICT profiles are required. In broad lines, these profiles are as follows:

Infrastructure administrators

These persons are responsible for integrating the HPC infrastructure in the data centre. They install the infrastructure in the data centre. They also install and manage the specific storage that is coupled to the HPC. In addition, they install and manage the internal network of the HPC and they connect the HPC into the university network and the Intranet. They are responsible for the security of the infrastructure and the daily monitoring of it. They participate in purchasing decisions on the integration of the infrastructure in the data centre.

System administrators

These persons are responsible for installing and administering the basic software on the HPC machines. This extends from the operating system to the scheduling software. They are responsible for the daily monitoring of HPC systems. They develop software for the efficient management of the HPC systems. They participate in purchasing decisions on the architecture of the HPC machine and the management software.

User support staff

These persons are responsible for basic user support. They man the first-line helpdesk and help users on their first acquaintance with the machine. They install the user software and help users efficiently use the machine. They are responsible for the documentation and provide basic training.

Academic or advanced support staff

These persons are responsible for optimisation of the user software on the HPC machines. For this they frequently work for a longer period with one user and give advanced training. These persons are responsible for adjusting the scheduler software so that it answers the needs of the users. They are responsible for setting up actions aimed at increasing the awareness of HPC and attracting new users. They participate in the purchasing decision on the user requirements and the benchmarks.

Project managers

These persons have the immediate management over the HPC teams or manage larger HPC projects. They are responsible for embedding the local HPC in the environment of the VSC. They are responsible for the coordination of HPC initiatives and user groups within their own institution. They are responsible for reporting to the funding providers. They have the final responsibility for purchasing files.

The percentage distribution of the deployment of the aforementioned profiles across the various institutes is as follows:

| | Infrastructure administration | System administration | Basic user support | Academic or advanced support | Project management |
|-----------------------|-------------------------------|-----------------------|--------------------|------------------------------|--------------------|
| Ghent University | 13% | 40% | 19% | 20% | 8% |
| University of Antwerp | 2% | 22% | 29% | 30% | 17% |
| VUB | 15% | 31% | 30% | 11% | 13% |
| University of Hasselt | 0% | 0% | 45% | 50% | 5% |
| KU Leuven | 15% | 31% | 19% | 20% | 13% |

Outreach

In addition, a large number of people devote part of their time to the outreach of HPC in Flanders, both to academic and other research centres and to the industry. They visit research groups and companies, and participate in various events.

In 2015, a great deal of attention went into the updating of the new website, the creation of documentation, and the preparation of promotional materials.

People from various profiles, ranging from employees responsible for user support to managers, contribute to the outreach effort.

For the VSC as a whole, 1.5 FTE were required to look after its outreach activities.

Advanced support

In order to provide advanced and academic support to the end-user, expertise in the domain is generally a plus. It is, however, impossible to accumulate domain expertise within each institution for a broad range of specific areas. That is why it is good to retain an overview of the various expertises that are present within the VSC so that users can call on advanced expertise across the institutions should they need it.

Computational Chemistry

3 persons with academic experience in this field

Physics

4 persons with academic experience in this field

Engineering

1 person with academic experience in this field

Mathematics (Numerical Methods)

4 persons with academic experience in this field

Computer science

9 persons with academic experience in this field

Staff list

| Name | Institution | % employed for HPC operations and support |
|-----------------------|-----------------------|---|
| Wouter Depypere | Ghent University | 100% |
| Stijn De Weirdt | Ghent University | 100% |
| Andy Georges | Ghent University | 100% |
| Kenneth Hoste | Ghent University | 100% |
| Ewan Higgs | Ghent University | 100% |
| Ewald Pauwels | Ghent University | 100% |
| Alvaro Simon Garcia | Ghent University | 100% |
| Jens Timmerman | Ghent University | 100% |
| Kenneth Waegeman | Ghent University | 100% |
| Danny Schellemans | Ghent University | 20% |
| Johan Van Camp | Ghent University | 30% |
| Luk Claes | Ghent University | 20% |
| Wim Waeyaert | Ghent University | 20% |
| Werend Brantegem | Ghent University | 10% |
| Bruno Cardon | Ghent University | 10% |
| Dieter Roefs | Ghent University | 50% |
| Stefan Becuwe | University of Antwerp | 100% |
| Franky Backeljauw | University of Antwerp | 100% |
| Bert Tijskens | University of Antwerp | 100% |
| Kurt Lust | University of Antwerp | 100% |
| Koen Decauwsemaecker | University of Antwerp | 10% |
| Muriel Dejonghe | University of Antwerp | 10% |
| Herwig Kersschot | University of Antwerp | 10% |
| Annie Cuyt | University of Antwerp | 5% |
| Stéphane Gérard | VUB | 100% |
| Balázs Hagató | VUB | 100% |
| Bart Verleye | VUB | 25% |
| Rosette Vandenbroucke | VUB | 50% |
| Olivier Devroede | VUB | 25% |
| Johan D'Hondt | VUB | 20% |
| Peter Van Rossem | VUB | 20% |
| Dirk Heyvaert | VUB | 30% |
| Philippe Leemans | VUB | 30% |
| Geert-Jan Bex | University of Hasselt | 100% |
| Jan Ooghe | KU Leuven | 90% |
| Ingrid Barcena | KU Leuven | 100% |
| Mag Selwa | KU Leuven | 100% |
| Martijn Oldenhof | KU Leuven | 100% |
| Leen van Rentergem | KU Leuven | 20% |
| Kim Paulissen | KU Leuven | 10% |
| Jo Vanvoorden | KU Leuven | 80% |
| Jo Vandeginste | KU Leuven | 100% |
| Tom Leuse | KU Leuven | 65% |
| Herman Moons | KU Leuven | 10% |
| Rudy Rys | KU Leuven | 20% |
| Tom Vanmierlo | KU Leuven | 100% |
| Sofie Pieraerd | KU Leuven | 10% |
| Philip Brusten | KU Leuven | 10% |
| Tom Vanhout | KU Leuven | 10% |

Computing on the VSC infrastructure

Allocation of Tier-1 computing time

There are a number of ways in which researchers can apply for computing time on Tier-1, as stipulated in the regulations.

For researchers from an academic institution, SOC, or equivalent research institution, the following access channels are available:

- Starting Grant
 - Maximum 100 node days of computing time
 - Can be applied for at any time, with quick turnaround time
 - To try out Tier-1 and perform benchmarks or software tests, as preparation for a full-scale project application
 - Free of charge
- Project Access
 - For allocations of 500-5000 node days of computing time
 - Project applications describe
 - the overall scientific project
 - the consortium that will carry out the computations
 - the funding channel
 - the computational tasks to be carried out (technical)
 - the software to be used
 - where appropriate, the scientific results obtained with previous Tier-1 project allocations
 - Project applications can be submitted at all times, but will be evaluated on 3 occasions during the year by the Tier-1 Allocation Board
 - Until the end of 2015: use subject to a fee

For the evaluation of Tier-1 project applications a 'Tier-1 Allocation Board' was installed. Four foreign experts were appointed:

- Walter Lioen, chairman (SURFsara, the Netherlands);
- Derek Groen (Computer Science, Brunel University London, UK);
- Sadaf Alam (CSCS, Switzerland);
- Nicole Audiffren (Cines, France).

Mrs Caroline Volckaert of the FWO coordinates the board. The HPC coordinators of the Flemish universities are invited to participate in the meetings as observers.

The board evaluates the applications and decides whether the requested computing time can be completely, partially or not allocated.

The 2015 regulations specify that academic researchers are to be charged a small portion of the costs for use of Tier-1: typically 5% of the full cost. The amount due for the used computing time is charged per Tier-1 project after the planned work has been carried out. Ghent University provides the necessary supporting documents and the amounts are collected by the Hercules Foundation.

In the course of 2015, however, this cost recovery was negatively evaluated by the HPC coordinators and the Tier-1 Allocation Board. The (limited) cost that is charged is nevertheless perceived as a significant obstacle for researchers. It also compromises access for less experienced research groups and new, challenging but high-risk research on the Tier-1 computing platform. On the other hand, the central effort involved in individual billing and justification is not commensurate with the income. For these reasons it was decided that, from 2016 onwards, costs would no longer be charged for Tier-1 projects allocated to academic researchers.

For industrial researchers, there are also two access channels for Tier-1 computing time:

- Exploratory Access
 - Maximum 100 node days of computing time
 - To try out the Tier-1 user environment or to perform benchmarks or software tests.
 - Free of charge
- Full Access
 - Companies can conclude an agreement with the Tier-1 housing institution and the Hercules Foundation/FWO to purchase computing time
 - Full cost charging of consumed computing time and used storage

The rates at which industrial users can purchase Tier-1 computing time have been laid down by the Board of Directors of the Hercules Foundation. In addition, industrial researchers can also gain access to Tier-1 as part of a research project that is carried out in collaboration with a Flemish university or institution of knowledge.

Allocation of Tier-2 computing time

Each university has its own procedure for the allocation of computing time on the Tier-2 infrastructure and may or may not charge a small portion of the costs to the academic researcher. For industrial/external users, all consumed computing time is always charged in full.

To gain access to one of the Tier-2 clusters in the four VSC hubs (Antwerp, Brussels, Ghent, Leuven), the user must have a VSC user ID, which can be requested at <https://account.vscentrum.be>. This website and the database also centralises all user information across the institutions, such as storages quota, membership of user groups, virtual organisations, etc.

Researchers of the University of Antwerp and its association have full free access to the Tier-2 infrastructure. Research groups can, however, make a financial contribution on a voluntary basis.

Researchers at the VUB can work on the HYDRA cluster after they have been granted access by the computer centre. The grid cluster is available on demand from the infrastructure administrator. Use of the Tier-2 infrastructure is free of charge.

Researchers of Ghent University and its association have full free access to the local Tier-2 infrastructure. Research groups can, however, make a financial contribution on a voluntary basis, with a (slightly) higher fair share as direct return-on-invest.

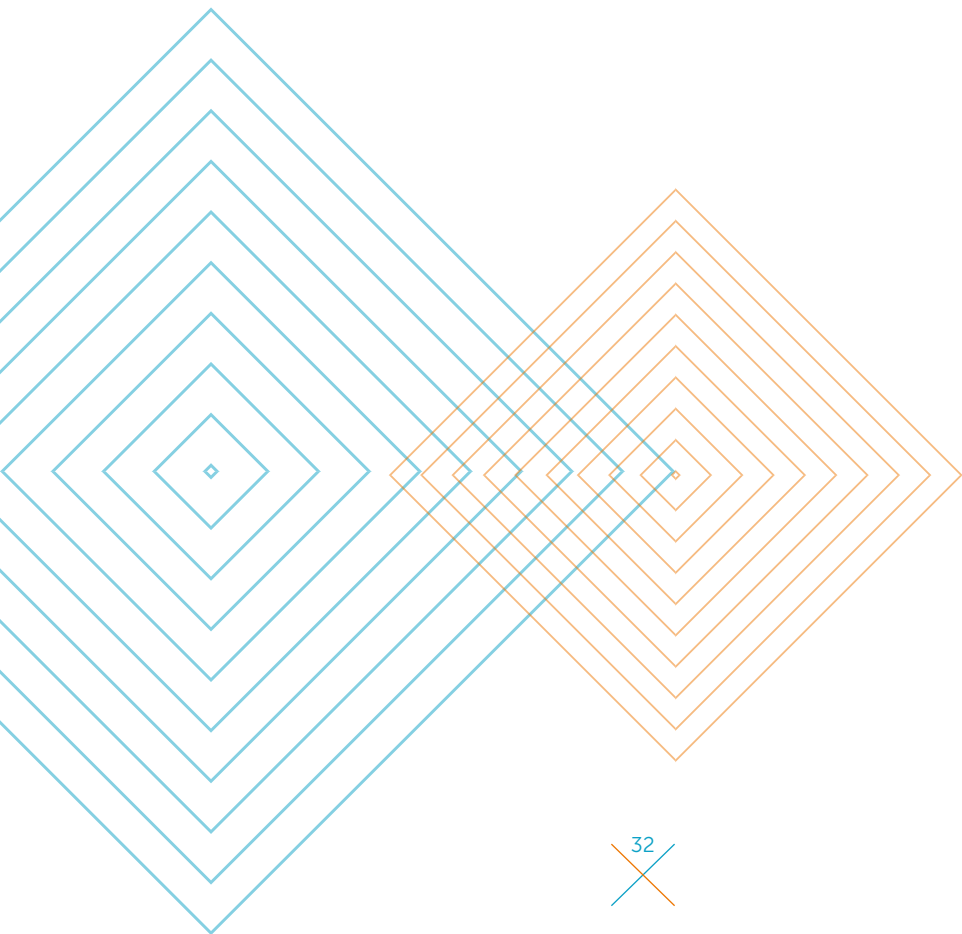
The clusters of KU Leuven/University of Hasselt use a credit accounting system that is incorporated in the scheduling software. New users receive computing time in order to become accustomed to the system and to carry out first tests. In this way, the barrier for researchers to switch to the Tier-2 infrastructure is kept as low as possible. Subsequently, credits can be applied for via a simple procedure and at minimum cost. The credits distribute the available computing time over various projects and have an empowering effect. When a computing job is carried out, the project to which the credits are to be charged, is specified. The principal researcher is the project manager. He/she can grant researchers access to the computing time and also monitor the used computing time.

Tier-1 Starting Grants / Exploratory Access

In 2015, 11 Starting Grants and 3 Exploratory Access projects were awarded.

| Starting Grants 2015 | | |
|----------------------|-----------------------|-----------------------------|
| Samuel Moors | VUB | Computational Chemistry |
| Stefan Weckx | VUB | Bioinformatics |
| Setareh Tasdighian | Ghent University | Bioinformatics |
| Nele Moelans | KU Leuven | Mechanical Engineering |
| Matthias Demuzere | KU Leuven | Environmental Modeling |
| Sam Vanden Broucke | KU Leuven | Environmental Modeling |
| Norbert Magyar | KU Leuven | Environmental Modeling |
| Jonas Bekaert | University of Antwerp | Computational Chemistry |
| Nikolaos Stergiannis | VUB | Environmental Modeling |
| Oriana De Vos | Ghent University | Computational Chemistry |
| Petar Marendic | VUB | Electromagnetic Engineering |

| Exploratory Access 2015 | |
|-------------------------|------------------------|
| FEops | Medical Engineering |
| Bekaert nv | Mechanical Engineering |
| Siemens | Mechanical Engineering |



Approved Tier-1 applications

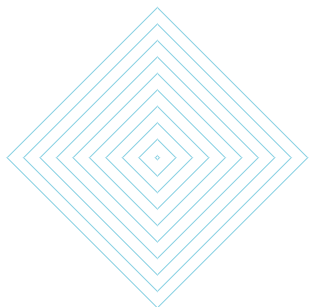
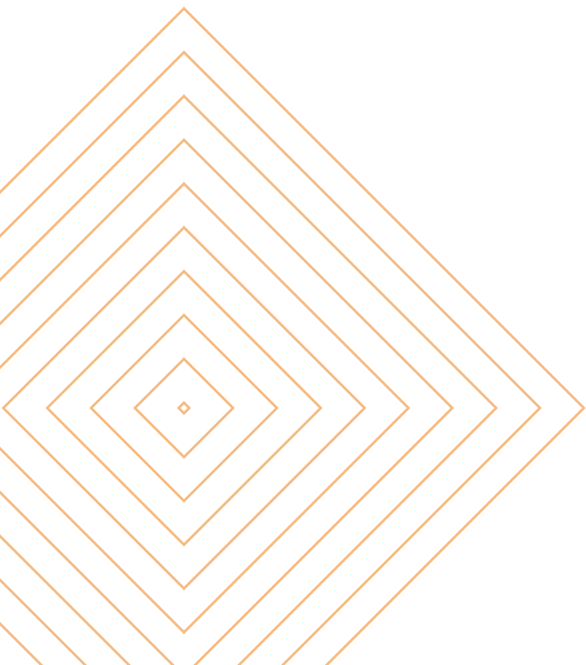
All applications approved in 2015, grouped per evaluation point, are listed below.

2 FEBRUARY 2015

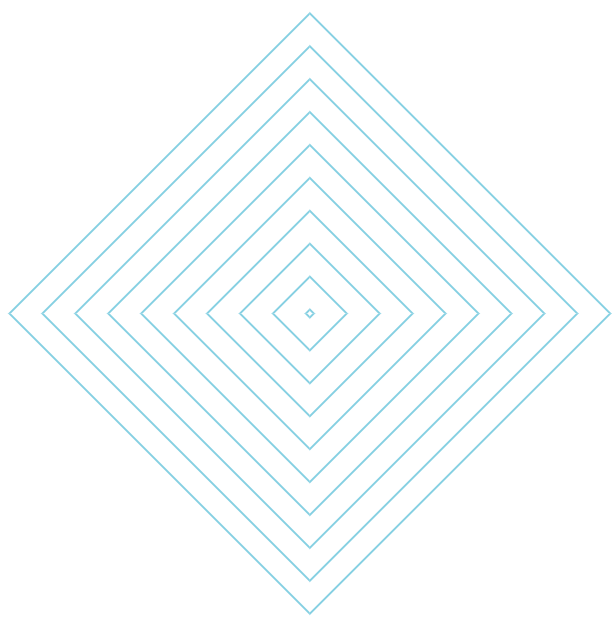
| Applicant | Host institution | Title | Science field | Allocated computing time (node days) | Allocated SCRATCH storage (TB) |
|--------------------|-----------------------|---|-------------------------|--------------------------------------|--------------------------------|
| Kurt Lejaeghere | Ghent University | Assessing the accuracy of a screened hybrid functional for property predictions of elemental solids | Computational Chemistry | 1,742 | 0.163 |
| Rony Keppens | KU Leuven | Solar and astrophysical dynamics: simulating to the resolution limits. | Environmental Modeling | 3,100 | 2.3 |
| Matthias Vandichel | Ghent University | Structural transformations during dehydroxylation reactions of UiO-66 type metal-organic frameworks; an extension with normal mode analysis | Computational Chemistry | 2,726 | 0.48 |
| Pieter Reyniers | Ghent University | Computational Fluid Dynamics based design of 3D reactors | Mechanical Engineering | 4,000 | 1 |
| Karel Dumon | Ghent University | Hunting for new quaternary Zintl phases of the 1:1:1:4 stoichiometry | Computational Chemistry | 1,000 | 1.843 |
| Johan Meyers | KU Leuven | Simulation and optimal control of wind-farm boundary layers | Environmental Modeling | 5,000 | 9.85 |
| Jan Jaeken | Ghent University | Ab initio prediction of acoustic anisotropy of Fe, Ni, and FeNi in the Earth's inner core | Computational Chemistry | 3,106 | 1.2 |
| Samuel Moors | VUB | Modeling the electrophilic aromatic substitution reaction with ab initio molecular dynamics | Computational Chemistry | 2,160 | 0.018 |
| Ben Brigou | VUB | Modeling the nucleophilic aromatic substitution reaction with ab initio molecular dynamics | Computational Chemistry | 2,160 | 0.018 |
| Piet Termonia | Ghent University | UGent EURO-CORDEX climate runs | Environmental Modeling | 10,000 | 0.3 |
| Marcel Ameloot | University of Hasselt | Atomistic picture of fluorescent probes into lipid bilayer membranes: probing lipid rafts | Computational Chemistry | 690 | 1.38 |

01 June 2015

| Applicant | Host institution | Title | Science field | Allocated computing time (node days) | Allocated SCRATCH storage (TB) |
|-------------------------------------|-----------------------|--|-----------------------------|--------------------------------------|--------------------------------|
| Vanpoucke Danny Eric Paul | University of Hasselt | The electronic structure of functionalized luminescent Metal-Organic Frameworks | Computational Chemistry | 2,905 | 0.109 |
| Thierry De Meyer | Ghent University | Accurate pKa calculations of pH-sensitive dye molecules | Computational Chemistry | 5,280 | 1 |
| Sam Vanden Broucke, Hendrik Wouters | KU Leuven | CORDEX.be: Combining Regional Downscaling Expertise in Belgium: CORDEX and beyond. Part I | Environmental Modeling | 1,650 | 3 |
| Jan Fostier | Ghent University | Resolving numerical instabilities when dealing with electromagnetic simulations involving billions of unknowns | Electromagnetic Engineering | 2,176 | 2 |
| Bart Partoens, Erik Neyts | University of Antwerp | Ab initio study of adsorption of polymer molecules on α -Cr ₂ O ₃ , α -Fe ₂ O ₃ , and α -Al ₂ O ₃ surfaces: the role of Van der Waals functionals | Computational Chemistry | 4,539 | 0.2 |
| Pieter Cnudde | Ghent University | Characterizing adsorption properties of C ₄ – C ₆ alkenes on H-ZSM-5 using molecular dynamics simulations | Computational Chemistry | 4,260 | 0.378 |
| Titus Crepain | Ghent University | Computational Discovery of Quaternary Zintl Phases | Computational Chemistry | 3,076 | 3.5 |
| Julianna Hajek | Ghent University | Unraveling dehydroxylation pathways on UiO-66 type systems with metadynamics | Computational Chemistry | 3,304 | 0.498 |
| Nele Moelans | KU Leuven | 3D microstructure evolution simulations of the effect of grain boundary diffusion on the growth velocity of intermetallic compound layers in Cu-Sn solder joints | Computational Chemistry | 2,250 | 0.02 |
| Pieter Reyniers | Ghent University | Computational Fluid Dynamics based design of 3D reactors (II) | Mechanical Engineering | 2,000 | 1 |
| Maere Steven | Ghent University | A stochastic birth-death model for evolution of gene family copy numbers along a phylogeny | Bioinformatics | 1,538 | 0.006 |
| Giovanni Lapenta | KU Leuven | KISIOPPE: Kinetic Simulations of the Planetary Plasma Environment | Environmental Modeling | 3,500 | 1.5 |



| Applicant | Host institution | Title | Science field | Allocated computing time (node days) | Allocated SCRATCH storage (TB) |
|-------------------------------------|-----------------------|---|-------------------------|--------------------------------------|--------------------------------|
| Dimitrios Millas, Bart Ripperda | KU Leuven | Outflow and Particle Evolution in Relativistic Astrophysics (OPERA) | Environmental Modeling | 2,500 | 3.2 |
| Rolando Saniz | University of Antwerp | Electronic properties of defect complexes in Sigma3 CIGS grain boundaries | Computational Chemistry | 4,140 | 0.065 |
| Kristof De Wispelaere | Ghent University | Confidential | Computational Chemistry | 1,400 | 0.125 |
| Jelle Wieme | Ghent University | Confidential | Computational Chemistry | 4,644 | 0.484 |
| Johan Meyers | KU Leuven | Simulation and optimization of wind farm boundary layers (II) | Environmental Modeling | 5,000 | 9.85 |
| Pieter Reyniers | Ghent University | Computational Fluid Dynamics based design of 3D reactors (III): enhanced reactors | Mechanical Engineering | 4,000 | 1.5 |
| Nikolaos Stergiannis | VUB | Confidential | Mechanical Engineering | 858 | 1 |
| Hendrik Wouters, Sam Vanden Broucke | KU Leuven | CORDEX.be: Combining Regional Downscaling Expertise in Belgium: CORDEX and beyond. Part II. | Environmental Modeling | 10,000 | 3 |
| Piet Termonia | Ghent University | UGent EURO-CORDEX climate runs II | Environmental Modeling | 5,000 | 42.000 |



Graphs on the use of Tier-1

Used CPU hours on Tier-1

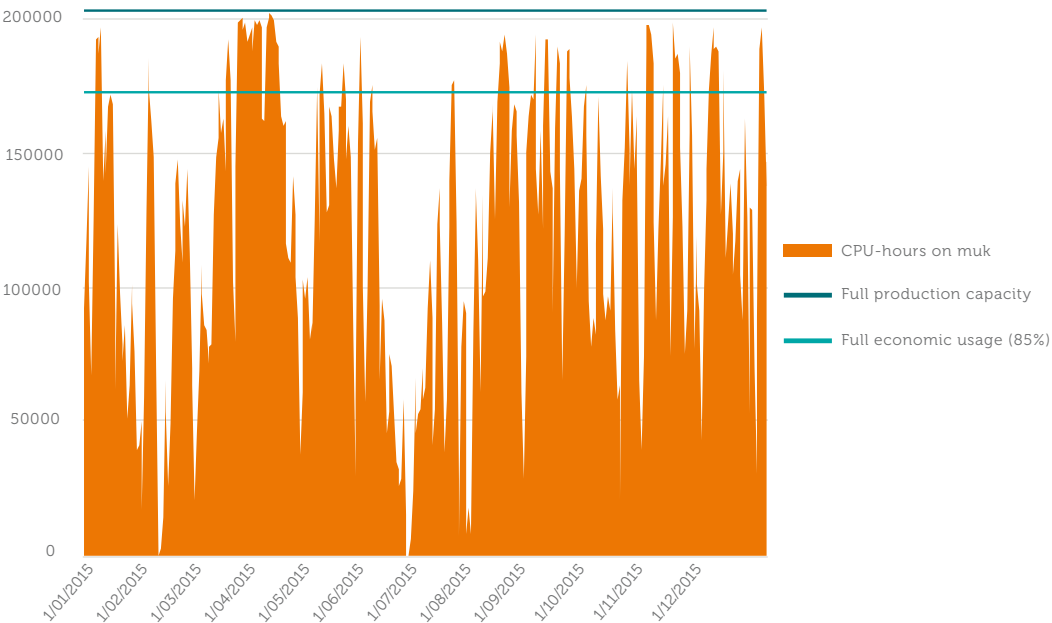


Figure 15
Use of Tier-1 cluster (muk), installed at Ghent University

The above graph presents an overview of the historical Tier-1 use in 2015. The complete Tier-1 use corresponds with 202,752 CPU hours per day, but 85% of this number is considered as ‘full economic’ use of the cluster. Both figures are shown in the graph.

The use of Tier-1 is subject to significant variations depending on the computing efforts of the users.

The visible dips in CPU hours used in 2015 are due to maintenance windows. During these periods, the machine was shut down completely and maintenance work carried out.

Allocated computing time in 2015 per institution

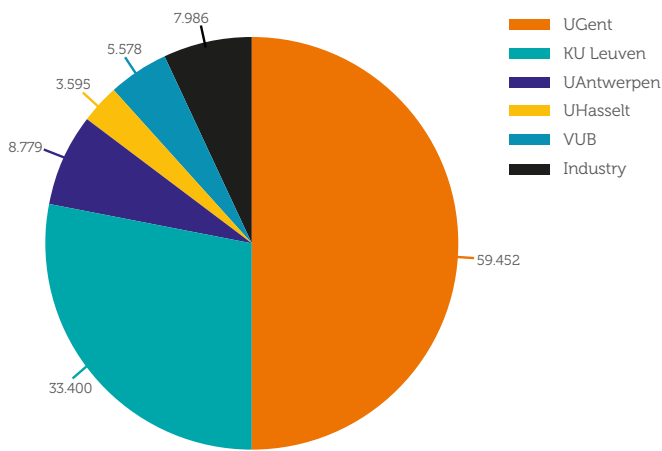


Figure 16
Distribution of allocated Tier-1 computing time in 2015 across the institutions expressed in node days

Allocated computing time in 2015 per science field

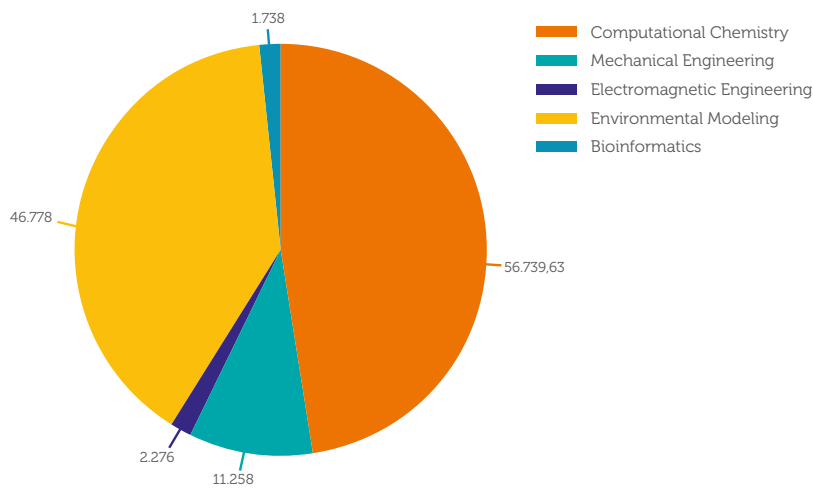


Figure 17
Distribution of allocated Tier-1 computing time in 2015 across the various science fields expressed in node days

The above graphs illustrate the distribution of the Tier-1 computing time across the various institutions and science fields. This is the Tier-1 computing time that was allocated by the Evaluation Committee in 2015. Node days were allocated not only to academic allocations. Almost 8000 node days were allocated to various industrial users of the Tier-1 infrastructure.

Areas of application are mainly in computational chemistry and climate modelling.

Outreach to Flemish companies

One of the missions entrusted to the Flemish Supercomputer Centre (VSC) under the HPC law, is informing companies and institutions from the non-profit sector about the added value of HPC in the development and optimisation of services and products. Another mission is to support them with the use of this new technology.

Services to companies

The range of services that VSC supply to companies are built on four pillars: consultancy, research collaboration, training and computing power.

Consultancy

VSC experts analyse the specific needs of the company and examine how supercomputing can offer added value for this company. The VSC offers a free intake interview to ascertain which benefits HPC can offer the company and which services in the VSC network best satisfy these needs.

Research collaboration

The VSC acts as HPC contact and can channel the question for research collaboration from a company (e.g. in the context of an R&D project).

Within the network, the VSC can bring the company into contact with a suitable top-level research partner in the Flemish academic landscape and act as intermediary.

Training

The VSC regularly organises basic training events that are also open to industrial users. Topics include Linux, (parallel) programming languages and paradigms, code optimisation, but also application-driven training such as materials science, computational fluid dynamics etc. Training customised for the end-user can also be provided.

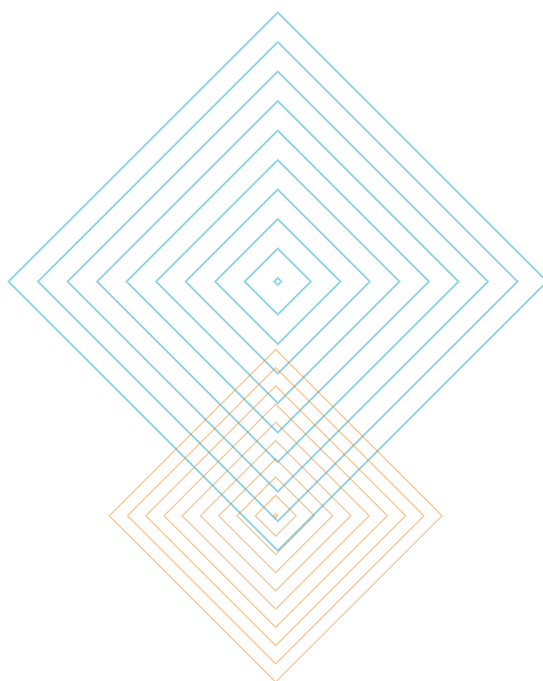
Computing power

Companies can, for internationally competitive prices, purchase computing time on the state-of-the-art supercomputing infrastructure within the VSC network. Users receive step-by-step support for starting computational tasks and a special helpdesk is ready to solve user-related questions and to assist the users in the installation of specific software.

Use of Tier-1 by companies

In 2015, two companies based in Flanders made regular use of Tier-1. The agreements for use were contractually concluded between the Hercules Foundation, Ghent University and the company involved. Several other companies have already shown interest in Tier-1 use, but are still in an exploratory phase.

The graph on the next page presents a (anonymous) view of the computing time used throughout the year.



Industry Tier-1 usage 2015

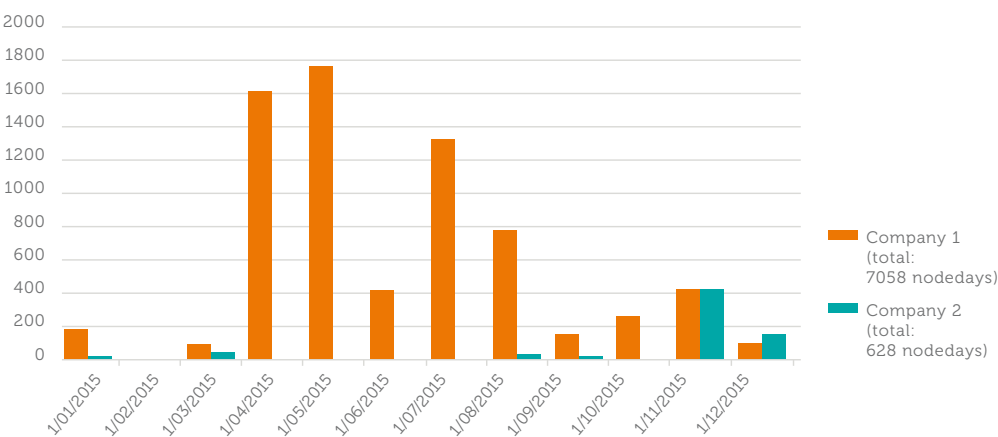


Figure 18
View of the computing time used throughout the year

Publication to companies and other knowledge institutes

The VSC Industry Day is one of the initiatives to reach out to the industry. On 27 January 2015, the VSC organised an event on industrial HPC applications at Technopolis (Mechelen). This successful event was aimed specifically at (potential) users of HPC in Flemish companies. The major objective was to make companies aware of the possibilities of large computing capacity and of the services provided by the VSC to develop new products more efficiently or improve existing ones.

A number of Flemish companies illustrated the importance of HPC for their operations by means of examples. Representatives of foreign HPC centers shared success stories about their collaboration with local companies. The VSC clarified the Flemish approach and explained the possibilities and access modalities for Flemish companies.

This event was well attended by participants from various industrial sectors, and proved an excellent occasion for networking between industrial and academic researchers. Furthermore, we could also welcome Philippe

Muyters, Flemish minister for work, economy, innovation and sport, who closed the event in a solemn note. About a hundred people signed up including employees of about twenty companies. Both large companies, consulting firms, SMEs and spin-offs of Flemish universities were represented. Many spontaneous contacts were made during the meeting. In this way, requests came up to get more information about VSC and to carry out tests on the Tier-1. Following this event, a number of companies were contacted to explore the possibilities of HPC and to clarify the support by VSC. Within the Industrial Board it was also discussed what the most appropriate approach is to transform “contacts” into “users of the VSC infrastructure” and to better disseminate the unique selling proposition of the VSC.

Also in 2015, several companies and other Flemish knowledge institutes were contacted by VSC partners for the purpose of assessing their HPC potential and promoting the use of supercomputing and the VSC services. These

contacts took the form of on-site user meetings and kick-start events to convince (potential) industrial users as optimally as possible of the added value of HPC and of the VSC for their company. In addition, a number of full-scale (mostly introductory) training sessions were organised.

Training and kick-start events:

- Bayer Cropscience, VSC info, 23/01/2015 and 30/01/2015 (Ghent University)
- Siemens, VSC info and kick-start on-site, 23/03/2015 (Ghent University)
- Umicore, VSC info on-site, 10/07/2015 (Ghent University)
- FEops, training on-site, 11/12/2015 (Ghent University)

User meetings:

- KMI, 16/02/2015 (Ghent University)
- J&J, hands-on on-site, 23/02/2015 (Ghent University)
- VITO, 3/09/2015 (University of Antwerp)
- FEops, 22/09/2015 (Ghent University)
- Bekaert NV, 18/11/2015 (Ghent University, FWO)

Other outreach events where companies were (indirectly) informed about HPC in Flanders:

- The VSC sponsored the Flemish Programming Competition edition 2015 to increase its name recognition among students with a keen interest in programming.

- On 17 March 2015, the core facility CalcUA (University of Antwerp) participated in "UAntwerpen backstage". On a continuous knowledge market, companies were introduced to the available facilities of University of Antwerp (and the VSC) and thus given the opportunity to establish contacts.



Training

Organisation and publication of training programmes

The VSC spends the necessary time on supporting and training researchers who make use of the infrastructure. It is important that calculations can be executed efficiently because this increases the scientific competitive position of the universities in the international research landscape.

Training organised by the VSC is intended not only for researchers attached to Flemish universities and the respective associates, but also for the researchers who work in the Strategic Research Centres, the Flemish scientific research institutes and the industry.

The training can be placed into four categories that indicate either the required background knowledge or the domain-specific subject involved:

1. Introductory
2. Intermediate
3. Advanced
4. Specialist courses & workshops

Introductory courses are intended for all users of the infrastructure and are highly recommended when one does not possess the required skills. These sessions are conducted by the local VSC staff. This offers researchers the opportunity to become acquainted with the people who answer the questions submitted to the helpdesk. This helps remove the impersonal and anonymous character that is part and parcel of email traffic.

To follow the sessions at the *intermediate* level, one must have followed the *introductory* courses so that the required background knowledge has been obtained. These sessions are also more specific in the subjects they deal with. The majority of these courses are intended for users who develop software themselves, either for computing-intensive applications, or for pre and post processing of data. This training is more specialised and intensive than the

introductory training, and is therefore not provided at every VSC site. Users are therefore encouraged to attend the training sessions at a different site.

Training at the *advanced* level requires more experience and is more domain-specific than the *intermediate* training. For these courses, VSC hires external instructors. Often they are connected to a PRACE Advanced Training Centre (PATC) or are from the industry. Only two or three such courses are organised each year. Some courses, however, do not fit in with any of the three above-mentioned levels. This may be because they are specific to a certain field or because they encompass everything from *introductory* to *advanced* level.

The training offer is published via the VSC website so that the information is available to all interested parties. The announcements are further distributed among the users of the infrastructure via internal mailing lists. Targeted mailings highlight specific training courses that could prove useful to a limited target group or to potential users.

A summary of the planned training courses is also included in each issue of VSC Echo, and a thematic issue on training is published once a year.

Training programme

An overview of the available training, listed per month, is given below:

January

- Linux introduction, 13 January, 7 hours, KU Leuven/University of Hasselt level: introductory
- Python for data processing, 20 & 21 January, 24 & 25 February, 16 hours, KU Leuven/University of Hasselt level: intermediate
- HPC@UGent introduction, 30 January, 6 hours, Ghent University level: introductory

February

- HPC@KU Leuven introduction, 11 February, 6 hours, KU Leuven/University of Hasselt level: introductory
- Linux for beginners, 12 March, 6 hours, Vrije Universiteit Brussel level: introductory
- Linux introduction, 26 February, 5 & 12 March, 9 hours, University of Antwerp level: introductory
- Python for data processing (part III & IV), 25 & 27 February, 8 hours, KU Leuven/University of Hasselt level: intermediate

March

- HPC@UGent introduction, 2 March, 6 hours, Ghent University level: introductory
- Python for data processing, 23, 25, 29 & 31 March, 16 hours, KU Leuven/University of Hasselt level: intermediate

April

- Introduction to HPC (for SCK-GEN researchers), 7 April, 3 hours, University of Antwerp location: SCK-GEN level: introductory
- Node-level performance engineering, 9 April, 14 hours trainer: dr. Georg Hager (RRZE, Erlangen, Germany) organisation: VSC, doctoral schools level: intermediate
- Spring School on Computational Tools for Materials Science, 13-17 April, 40 hours, Ghent University organisation: VSC, doctoral schools, Center for Molecular modelling (CMM) - Ghent University level: specialist
- Message Passing Interface (MPI), 22 April, 7 hours, Ghent University trainer: prof. Dr. Jan Fostier organisation: VSC, doctoral schools level: intermediate
- Introduction to R: an open source statistical toolbox, 23 & 24 April, 8 hours, Vrije Universiteit Brussel level: introductory
- Lunchbox session Cerebro, 23 April, 2 hours, KU Leuven/University of Hasselt level: introductory

- Guest lecture on HPC (ikv Information Technology and Data Processing), 28 April, 4 hours, Ghent University level: introductory
- Lunchbox session: new Thinking components — Spring 2015, 2 hours, 28 April, KU Leuven/University of Hasselt level: introductory

May

- Modern Fortran, 12 May, 4 hours level: intermediate
- Guest lecture on HPC (for HOWest researchers), 12 May, 4 hours, Ghent University level: introductory
- Migrating old to modern Fortran code, 20 May, 7 hours trainer: dr. Reinhold Bader (LRZ, Garching, Germany) organisation: VSC, doctoral schools level: intermediate
- Introduction to multithreading and OpenMP, 21 & 22 May, 14 hours, Ghent University trainer: dr. Reinhold Bader (LRZ, Garching, Germany) organisation: VSC, doctoral schools level: intermediate
- GUI launcher tutorial, 29 May, 1 hour, University of Antwerp level: introductory
- Getting started with high-performance computing, 27-29 May, 1-3 June, 36 hours, Ghent University level: introductory

October

- Matlab, 1, 2, 8, 9, 15 & 16 October, 24 hours, University of Leuven level: introductory
- HPC@UGent introduction, 5 October, 6 hours, Ghent University level: introductory
- HPC@KU Leuven introduction, 8 October, 6 hours, KU Leuven/University of Hasselt level: introductory
- HPC@UAntwerpen introduction, 12 October, 4 hours, University of Antwerp level: introductory
- Linux introduction, 16 October, 7 hours, KU Leuven/University of Hasselt level: introductory

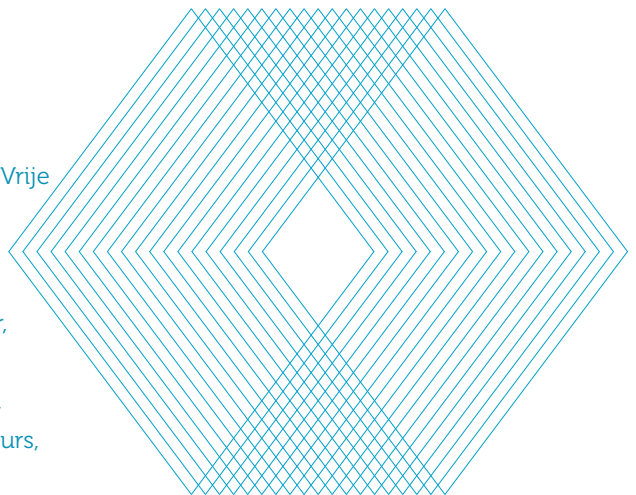
- Lunchbox session visualization HPC@KU Leuven, 27 October, 2 hours, KU Leuven/University of Hasselt
level: introductory
- Python course, 29 & 30 October, 10 & 11 November, 16 hours, KU Leuven/University of Hasselt
level: introductory
- Version control with git, 4 December, 3 hours, University of Hasselt
level: introductory
- HPC tips & tricks 3: using checkpointing, 11 December, 2 hours, University of Antwerp
level: intermediate

November

- HPC@KU Leuven introduction, 5 November, 6 hours, KU Leuven
level: introductory
- Linux for beginners, 6 November, 6 hours, Vrije Universiteit Brussel
level: introductory
- HPC@UGent introduction, 10 November, 6 hours, Ghent University
level: introductory
- Linux@UHasselt introduction, 13 November, 4 hours, University of Hasselt
level: introductory
- MPI course, 17 & 19 November, 15 hours, VSC
location: KU Leuven
based on PATC course by dr. Rolf Rabenseifner (HLRS, Stuttgart, Germany)
level: intermediate
- OpenMP, 24 November, 7 hours, VSC
location: KU Leuven
based on PATC course by dr. Rolf Rabenseifner (HLRS, Stuttgart, Germany)
level: intermediate
- Info session: version control with subversion/git, 26 November, 3 hours, KU Leuven
level: introductory
- HPC@UHasselt introduction, 27 November, 4 hours, University of Hasselt
level: introductory
- Introduction to High Performance Computing, 27 November, 6 hours, Vrije Universiteit Brussel
level: introductory

December

- Debugging techniques, 1 December, 4 hours, KU Leuven
level: introductory
- Lunchbox session storage overview HPC@KU Leuven, 3 December, 2 hours, KU Leuven/University of Hasselt
level: introductory



Communication and events

VSC ECHO

VSC Echo is the newsletter of the VSC and is published three times a year. In 2015, the VSC Echo appeared in mid-January, late June and late September. The January 2015 issue, VSC Echo 6, was focused on the Industry Day, VSC Echo 7 announced the purchase of a new Tier-1 and also advertised the new VSC website. The September issue, VSC Echo 8, was traditionally devoted to the VSC training programme.

Each VSC Echo also contains news in connection with the use of Tier-1. Thus, information was provided about the amendments to the regulations, about the submission of project proposals around the use of computing time on Tier-1, about the closing dates for submitting proposals etc. The VSC Echo is sent electronically to more than 2,000 addresses and a paper version is available at events, meetings etc. as well as on the VSC website.

User Day 2015

The second VSC User Day took place on 30 November 2015. This edition was held at the University of Antwerp. More than 90 participants had registered for the varied programme put together by the User Committee. Both the morning and afternoon sessions were built around the same pattern: a plenary session followed by a choice from 4 workshops. The following topics were discussed in the workshops: "VSC for starters", "Specialized Tier-2 infrastructure: shared memory", "Big data" and "Cloud and grid access". The participants were interested in all four workshops. In his lecture "High performance and multiscale computing: blood, clay, stars and humans", Derek Groen explained "multiscale computing" and demonstrated how he applied this technique in different areas of application. In the afternoon, Johan Meyers introduced us to simulations of wind farms in "High-performance computing of wind farms in the atmospheric boundary layer". Subsequently, he presented us with a view of the in-house developed code and its parallelisation. At the end, researchers presented their HPC related research in a poster session, for which the audience was warmed up via one-minute presentations. This approach also explained why so many participants were clearly interested in the numerous posters. Discussions were continued while enjoying a refreshing drink. The completed evaluation forms were unanimously positive.



Participation in (inter)national events

Participation in national events

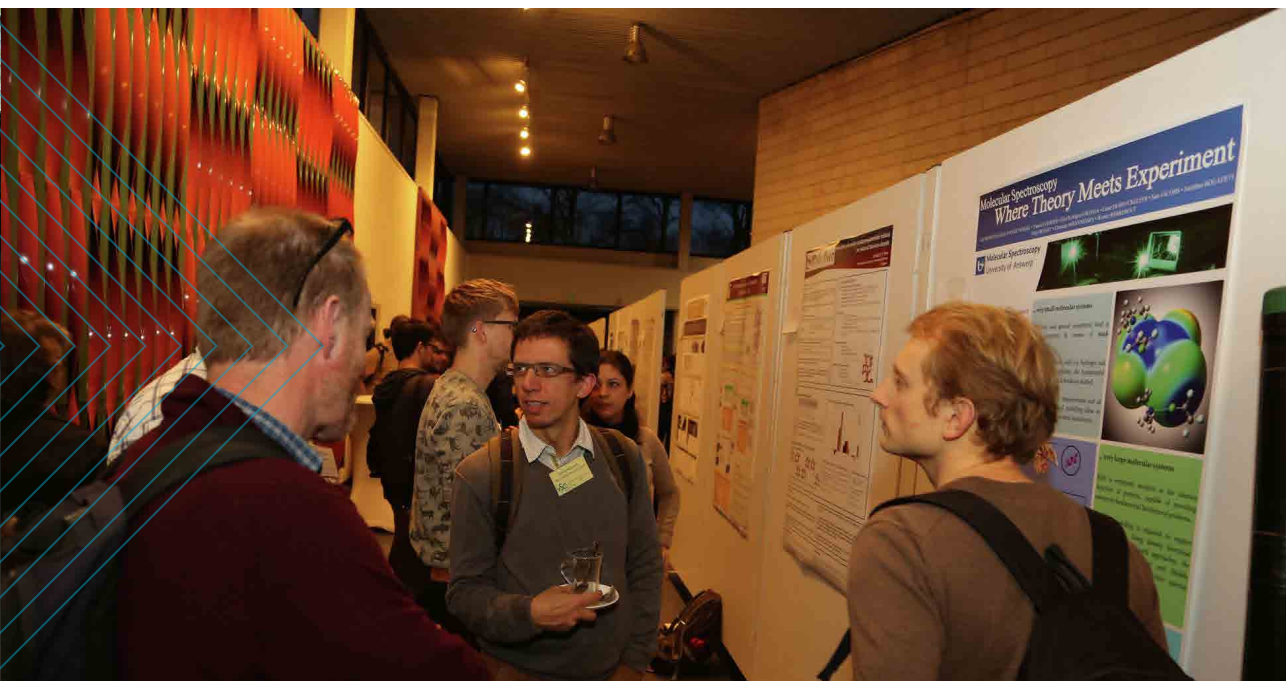
Organised by VSC

- Tacc_Stats and xalt – Ghent University
29 January 2015 – Ghent University
Attended by Engelbert Tijksens, Ingrid Barcena, Geert Jan Bex, Andy Georges, Kenneth Hoste,
- Tools for Computational Materials – Ghent University
13-17 April 2015 – Ghent University
Attended by Engelbert Tijksens, Geert Jan Bex, Jens Timmerman
- Migrating old to modern Fortran code – KU Leuven
20 May 2015 – Leuven
Attended by Engelbert Tijksens
- Introduction to multithreading and OpenMP – KU Leuven
21-22 May 2015 – Leuven
Attended by Engelbert Tijksens, Andy Georges
- Intensive course on computational and theoretical chemistry for Erasmus Mundus Masters
Department of Chemistry KU Leuven
9 September 2015 – Leuven
Attended by Ingrid Barcena

- Data science in practice – Computer Sciences KU Leuven
14-15 September 2015 – Leuven
Attended by Mag Selwa, Martijn Oldenhof

Organised by other organisations

- Big on Data, FLAMES annual meeting 2015
13 May 2015 – Ghent
Hands-on session 'Using the Flemish supercomputer by the Flemish Supercomputer Center' organised by VSC
Attended by Ewan Higgs, Andy Georges, Kenneth Hoste, Stijn De Weirtdt, Jens Timmerman, Kenneth Waegeman, Alvaro Simon Garcia, Geert Jan Bex
- Aviation Research Day
19 October 2015 – Leuven
Attended by Geert Jan Bex, Ingrid Barcena, Jan Ooghe
- Belnet networking conference
22 October 2015 – Brussels
Attended by Stefan Becuwe, Kurt Lust
- e-Infrastructures in Belgium day
14 December 2015 – Brussels
Lecture 'Flemish Supercomputer Center: Tier-1 services in Flanders' presented by Ewald Pauwels
Lecture 'VSC: The Flemish supercomputing infrastructure' presented by Stefan Becuwe
Attended by Stefan Becuwe, Stéphane Gérard, Kurt Lust, Jan Ooghe, Ewald Pauwels, Rosette Vandenbroucke, Bart Verleye



International collaboration

PRACE

The VSC is, via the Belgian membership, part of the PRACE happening. PRACE offers the possibility of using Tier-0 computing time. Access to Tier-0 computing time is organised through calls for submissions of project proposals. These proposals are assessed according to 'excellent science' norms. The projects that are ranked highest receive the requested computing time. Flemish researchers are made aware of the existence of these calls through notifications on the VSC website and announcements in the VSC Echo. PRACE also offers interesting training courses that are promoted by the VSC.

EGI

The VSC is actively present at the European Grid Infrastructure event (EGI). The VUB grid cluster is part of EGI and offers in this way the possibility for researchers from throughout Flanders to use this European computing infrastructure. Primarily high energy physicists from the University of Antwerp, Ghent University and the VUB make use of this. The research group "Icecube" has also decided to use this computing infrastructure in replacement of their own computing resources. EG has also set up a "federated cloud" which can also be accessed by the VSC via the VUB cloud. The first users interested in this computing facility are researchers from the humanities.

SESAME Net

The VSC is partner in the SESAME-NET project, that was awarded to the consortium within the Horizon 2020 programme of the EU. SESAME Net stands for 'Supercomputing Expertise for Small and Medium Enterprise Network' and its main objectives are: supporting, expanding and promoting a network of HPC knowledge and HPC experience in Europe. It is also

responsible for the dispersal of best practices around HPC usage by the industry. The primary target group are SMEs.

One of the particular characteristics of SESAME Net is the consortium: it consists of a mix of national and regional HPC groups supplemented with private partners. There are 15 partners from 13 EU countries: HPC-Wales (UK), ICHEC (Ireland), Fraunhofer institute (Germany), PSNC (Poland), GRNET (Greece), CESGA (Spain), PT Cloud (Portugal), IT4Innovations (Czech Republic), Yotta (Croatia), UVT (Romania), IICT (Bulgaria), RBI (Croatia), FWO/VSC (Belgium) and Vilnius University (Lithuania).

The project was officially launched on 1 June 2015 and runs for a period of 2 years. The VSC is mainly active in work package 4: Awareness Raising. In the period June-December there were 2 physical meetings (in Brussels and Lisbon) and a number of conference calls. The general structure is in place and there are clear agreements regarding the way of working and quality control. For work package 4, successful HPC user stories at SMEs have been collected and posted on the website. The preparation for an SME survey regarding their needs and expectations (in terms of HPC) has been launched, as have the preparations for the first newsletter.

Ward Poelmans (FWO) is temporarily in charge of these project resources (until November 2016) and responsible for all SESAME Net-related tasks. In this connection, he proactively contacts potentially interested companies, and monitors them when they effectively make the switch and use the VSC services.

Website: <http://sesamenet.eu>

Contacts with other HPC centres

The VSC regularly maintains contact with other HPC centres not only to keep abreast of developments in HPC, but also to exchange best practices. In fact, many HPC centres worldwide use various hard- and software solutions for resolving recurrent problems. Exchanging such information is of high importance for the operation of each HPC centre.

- Texas Advanced Computing Center (TACC, US)
29 January - 3 February – Ghent
Consultation with Robert McLay
- Jülich Supercomputing Center (Germany)
28-29 April 2015 – Ghent
Consultation with Bernd Mohr, Marcus Geimer
- Rutherford Appleton Laboratory (UK)
11-13 August 2015 – Daresbury, UK
On-site consultation, attended by Wouter Depypere, Kenneth Waegeman
- Consultation with delegation of Cuban universities
24 September, 7 October 2015 – Ghent
Contact with University of Informatic Sciences (UCI, Havana), Central University of Las Villas (Santa Clara), University of Santiago de Cuba
- 3TU.Datacentrum
23 October 2015 – Delft
Attended by Ewan Higgs

Several international contacts took place in the context of the cooperation on EasyBuild (<http://hpcugent.github.io/easybuild/>). This is a 'killer tech' software solution for installing scientific software on HPC systems in an easy, efficient and reproducible manner. Initially, this software was developed within the VSC. Today, however, many HPC centres throughout the world have come to appreciate the importance of this open source tool and are increasingly participating in the further development and maintenance of this code.

- 8th EasyBuild hackathon
9-11 February 2015 – Basel, Switzerland
<https://github.com/hpcugent/easybuild/wiki/8th-EasyBuild-hackathon>
Co-organised by Kenneth Hoste, Jens Timmerman
- 9th EasyBuild hackathon
4-5 May 2015 – Espoo, Finland
Part of the Nordic e-Infrastructure Collaboration workshop NeIC 2015
<https://github.com/hpcugent/easybuild/wiki/9th-EasyBuild-hackathon>
Co-organised by Kenneth Hoste

- Internal hackathon @ CSCS (Swiss National Supercomputing Centre)
7-9 September 2015
Co-organised by Kenneth Hoste
- 10th EasyBuild hackathon
11-13 November 2015 – TACC Austin Texas, USA
<https://github.com/hpcugent/easybuild/wiki/10th-EasyBuild-hackathon>
Co-organised by Kenneth Hoste

Participation in conferences and workshops

To enhance the international visibility of the VSC, to collect information that is useful for the further expansion of the HPC capacity in Flanders and to set up international partnerships, the employees of the VSC participate in international conferences and scientific meetings. A summary is given below:

- FOSDEM 2015
31 January - 1 February 2015 – Brussels
Attended by Kenneth Hoste, Andy Georges, Alvaro Simon Garcia, Ewan Higgs
- 19th Quattor Workshop
3-5 March 2015 – Grenoble, France
Attended by Kenneth Waegeman, Stijn De Weirdt, Wouter Depypere (Ghent University)
- Parallel I/O – Jülich Prace
16-18 March 2015 – Jülich, Germany
Attended by Geert Jan Bex
- Intel EMEA HPC Roundtable
17-18 March 2015 – Oxford, UK
Attended by Ingrid Barcena and Jan Ooghe
- Storage Expo / info security
25 March 2015 – Brussels
Attended by Jens Timmerman, Wouter Depypere
- The Sixth International Conference on Cloud Computing, GRIDs, and Virtualization
22-27 March 2015 – Nice, France
Attended by Rosette Vandenbroucke

- Big Data Science Symposium (FLAMES)
11 May 2015 – Ghent
Contribution to panel discussion by
Ewald Pauwels
- EGI Conference 2015
18-22 May 2015 – Lisbon, Portugal
Attended by Stéphane Gérard and Ro-
sette Vandenbroucke
- Intel Phi dev conference
6-7 May 2015 – Munich, Germany
Attended by Martijn Oldenhof
- Intel Phi dev conference
17-18 June 2015 – Amsterdam, Nether-
lands
Attended by Kurt Lust
- Summer school visualisation Hartree
Centre
14-19 June 2015 – Warrington, UK
Attended by Geert Jan Bex
- ISC 2015
12-16 July 2015 – Frankfurt Am Main,
Germany
Birds-of-a-feather session 'Getting Scien-
tific Software Installed: Tools & Best Prac-
tices' Presented by Andy Georges
Attended by Jens Timmerman
- IEEE eScience conference 2015
31 August, 1-4 September 2015 – Munich,
Germany
Attended by Rosette Vandenbroucke
- 20th Quattor Workshop
29 September – 1 October 2015 – Paris,
France
Attended by Stijn De Weirtdt, Kenneth
Waegeman
- ICT 2015
19-22 October 2015 – Lisbon, Portugal
Attended by Rosette Vandenbroucke
- OpenNebulaConf 2015
20-22 October 2015 – Barcelona, Spain
Lecture 'OpenNebula Automated De-
ployments with Quattor Toolkit' by Al-
varo Simon Garcia
Attended by Andy Georges and Alvaro
Simon Garcia
- Advanced MPI @ EPCC
28-29 October 2015 – Edinburgh, UK
Attended by Geert Jan Bex
- 29th Large Installation System Adminis-
tration conference (LISA15)
8-13 November 2015 – Washington DC,
United States
Attended by Andy Georges
- EGI Community Forum 2015
10-13 November 2015 – Bari, Italy
Attended by Stéphane Gérard, Bart Verl-
eye and Rosette Vandenbroucke
- Supercomputing Austin
15-20 November 2015 – TACC Austin
Texas, USA
Birds-of-a-feather session 'Getting Scien-
tific Software Installed: Tools & Best Prac-
tices' co-presented by Kenneth Hoste
Attended by Ingrid Barcena, Jan Ooghe,
Ewan Higgs, Kenneth Hoste

VSC success stories

Bekaert nv: modeling wire manufacturing

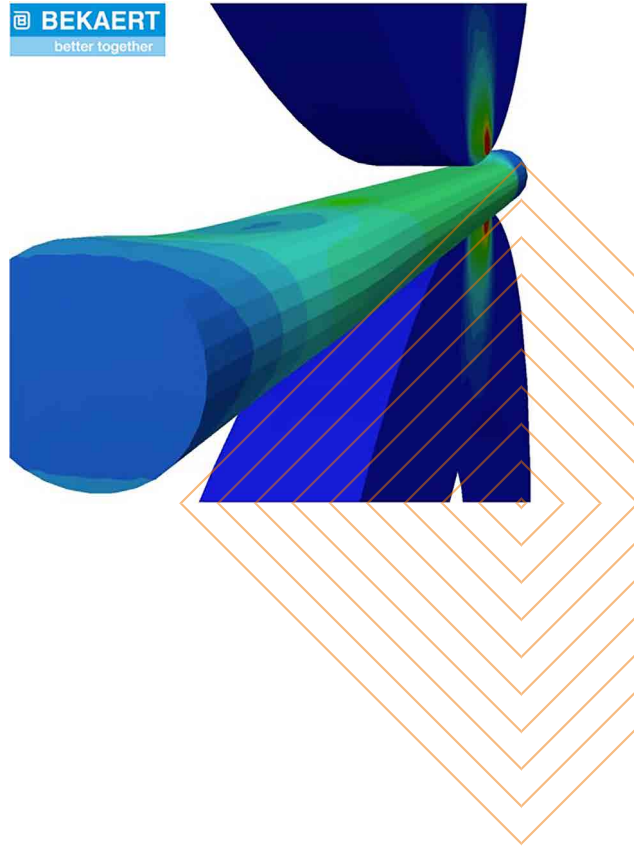
Bekaert is a world market and technology leader in steel wire transformation and coating technologies. Headquartered in Flanders, it is a global company with almost 30.000 employees worldwide. Bekaert is a prime supplier of steel cord products for tire reinforcement and steel fibre for concrete reinforcements. But it offers a very wide range of advanced steel wire products for other applications and to many sectors.

Peter De Jaeger, Team Leader Modelling, explains how Bekaert benefits from supercomputing:

"We use computational models to predict the behaviour of steel wire during different transformation processes (e.g. wire rolling, wire drawing, rope manufacturing, ...). Such calculations are much faster and more economic than relying on physical tests on proofing samples. In this way, supercomputing allows us to drastically enhance the speed of product development and improve development processes."

"But this modelling approach requires proper software implementation and ample computational resources." For both, Bekaert relies on the services of the VSC. A tailor-made version of the OpenFOAM-extend software was installed and made available on all clusters by the VSC support team. All Bekaert's computational models now run in an efficient manner on the Tier-1 and Tier-2 infrastructure of the VSC.

Peter De Jaeger: "The VSC team offers world-class supported computational infrastructure which makes high performance computing feasible from an industry perspective."



Evolutionary Systems Biology lab (Ghent University, VIB)

The Evolutionary Systems Biology lab is a young and dynamic research laboratory at the Plant Systems Biology department of VIB and Ghent University, led by Prof. Dr. Ir. Steven Maere. Its main goal is to understand how plant developmental systems work and how they evolve. Dr. Jayson Gutiérrez is a postdoc at the lab and describes his research.

“The way in which cellular organisms behave is determined by a set of genes that interact with each other in a so-called regulatory network. The main components of this network are DNA-binding proteins, which have evolved to fully control the expression of genetic information into the phenotype. Over evolutionary time scales, changes in the regulatory wiring of these networks provide a major source of functional innovation, potentially mediating the adaptation of organisms to changing environmental conditions.”

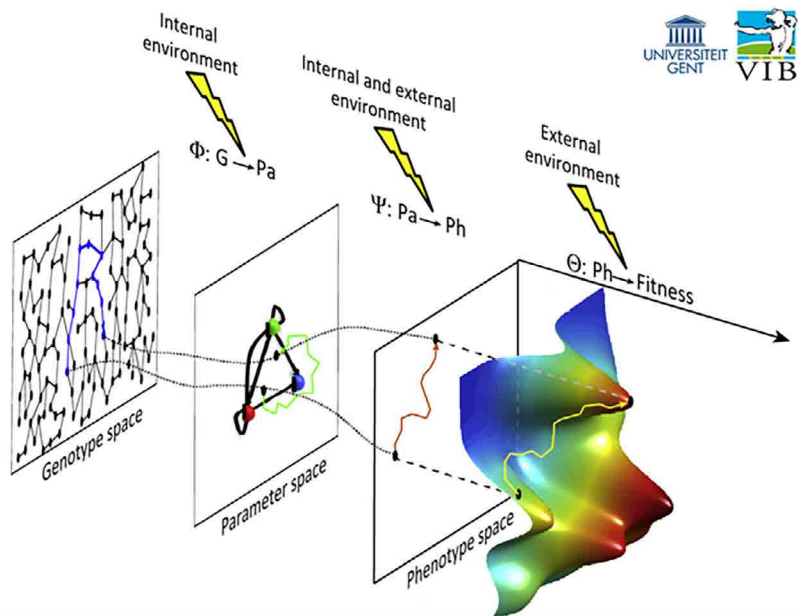
Dr. Gutiérrez is one of the researchers in Prof. Maere’s group that try to understand these regulatory networks at the mechanistic level by developing an elaborate computational model.

“Using different types of evolutionary algorithms, and by relying on the supercomputing infrastructure of the VSC, we have gathered massive amounts of information on how the network model reacts. This allows us to test existing hypotheses, and to formulate new ones. Our simulation results offer exciting new insights on the evolution and function of complex biological systems.”

But that is not all. A fully functioning mechanistic network model of this kind could eventually be used as a computer-aided design tool for synthetic biology, an interdisciplinary field that relies on genetic engineering and systems biology-inspired modeling approaches to engineer different types of biological circuits, including regulatory networks.

“For instance, our model could potentially give cues on how to design regulatory networks with the ability to perform specific biological tasks, such as the regulation of the expression of particular proteins whose intracellular concentration is required to change periodically over time.”

“The execution of this project would not have been possible without the use of the massive computer resources provided by the VSC infrastructure and the fantastic IT support!”



The VSC work plan 2016

As from 2016 the activities of the Hercules Foundation will be taken over by the Research Foundation-Flanders (FWO). The FWO will ensure the continuity of all tasks that were previously the responsibility of the Hercules Foundation. The Flemish Supercomputer Centre remains a partnership between the five Flemish universities and the FWO. Operationally, this centre is controlled by the VSC Steering Group which is composed of FWO staff and the HPC coordinators of the universities. The HPC law stipulates that the FWO will continue to be responsible for the financing of the large computing infrastructure for research and innovation and the management of Tier-1.

In 2016, we will continue to build on the initiatives that have already been launched in recent years. In addition, however, a significant number of new activities are being planned:

Financing of recurrent costs

As in 2015, in 2016 the FWO has an amount of €4 million for the structural financing of:

- 17 FTE of employees. In addition to the technical operation of Tier-1, these employees are responsible for the training and support of users of both Tier-2 and Tier-1;
- part of the operating and investment costs of the Tier-1 and Tier-2 computers.
- For this the FWO concludes annual grant agreements with the universities. Apart from the grants allocated by the FWO, the universities contribute from their own resources to the financing of additional staff, operating and accommodation costs and investments.

Publication, training and support

To publish the available possibilities, to inform (potential) users, and to create a user community:

- the third HPC User Day is organised in the second half of 2016;
- the VSC Echo newsletter is periodically distributed electronically on a large scale;
- a brochure aimed at industrial users is put together;

- a launch event for the second Tier-1 will be organised in October 2016.

The VSC offers training solutions tailored to the level and the needs of its users. Both standard training courses and more specialised courses will be organised. A summary of these courses is regularly disseminated via the VSC website. Furthermore, users are informed about the training organised by foreign centres and in which they can participate.

The training courses organised in the context of the VSC are, wherever possible, also open to users from the industry.

User support ranges from the helpdesk for solving small, routine problems to individual coaching of researchers by experts who are well positioned to optimise software and use software packages at an advanced level.

Allocation and management of Tier-1 computing time

Based on an evaluation, the regulations for applications for the use of the Flemish Supercomputer were amended in a number of areas. The new version takes effect on 1 January 2016. The appointment of the foreign members of the Evaluation Board was renewed.

As in 2015, applications will be evaluated at three cut-off dates:

February 1, June 6 and October 3.

HPC and industry

One of the missions entrusted to the VSC under the HPC law, is to inform companies and institutions from the non-profit sector about the importance of HPC for the development of new and the improvement of existing services and products, and to support them with the use of this new technology.

Since 2014, the first contracts with Flemish companies were signed for the purchase of computing time. To inform companies about the possibilities and to illustrate these via concrete cases and in an intelligible manner, a new event has been planned for 2016. Testimonials of Flemish companies who have already found their way to the VSC, but also speakers from foreign supercomputer centres having extensive experience in cooperation with industry, will participate in this event.

The VSC will also participate in the European Horizon 2020 SESAME-Net project. In SESAME-Net (Supercomputing Expertise for Small and

Medium Enterprises), the added value of super-computing for SMEs is promoted and access to HPC infrastructure facilitated.

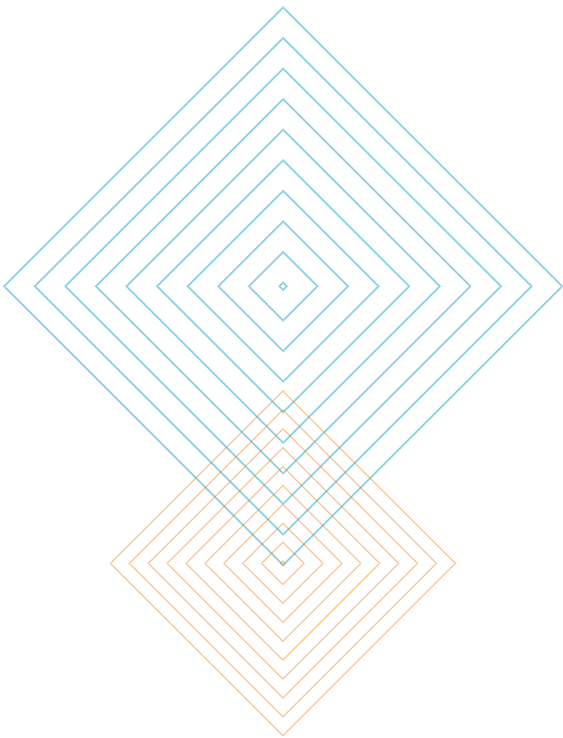
The second Flemish Tier-1

In 2014, the Hercules Foundation decided to award the accommodation and the technical operation of the second Flemish Tier-1 to KU Leuven. The company NEC was selected to build the machine through a public tender procedure.

The new machine will be installed at KU Leuven in the middle of 2016. It will be one of the 200 fastest computers in the world. A launch event is planned for October 2016 and several initiatives will be developed to raise the awareness of the new supercomputer.

Improving the service

Since 2014, the HPC coordinators have defined a number of projects which will be prioritised to improve the Tier-1 and Tier-2 services. Some projects are completed within one year, others are still ongoing. For 2016 a number of additional projects are being set up. In March 2016, a second all-hands meeting will be organised in which all persons responsible at the universities for operation of the HPC infrastructure and user support, will participate. On that day, the status of the ongoing projects and the planning will be discussed and working groups will be appointed for their implementation.



Colophon

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

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