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DEPARTMENT ICT

HPC-UGENT USER MEETING 2017

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

15/12/2017

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VSC Vlaams Supercomputer Centrum

PROGRAM

- (13h00: Optional tour of datacenter)
- 14h00: Welcoming address
- 14h15: Overview of HPC-UGent, VSC, future plans
- 14h45: Review of user poll results, Q&A
- 15h15: User in the spotlight - Pieter Reyniers, LCT
- 15h45: Slots for 1-minute poster presentations
- 16h15 - 18h00 Networking reception & poster session

ABOUT HPC-UGENT

Part of ICT department, Infrastructure office

Mission

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

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ABOUT HPC-UGENT

Personnel

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

Alvaro Simon Garcia
Cloud, user support

Andy Georges
Sysadmin, integration

Ewald Pauwels
Team lead

Jens Timmerman
Security, sysadmin

Kenneth Hoste
User support

Kenneth Waegeman
Sysadmin, storage

Stijn De Weirdt
Technical lead

Wouter Depypere
Sysadmin

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Always mail hpc@ugent.be

HPC-UGENT INFRASTRUCTURE

Storage

$VSC_HOME	35 TB	
$VSC_DATA	702 TB (1 PB)	2017-Q2
$VSC_SCRATCH $VSC_SCRATCH_KYUKON	1 PB	2017-Q2
$VSC_SCRATCH_PHANPY	35 TB SSD	

Compute clusters





	#nodes	CPU	Mem/node	Diskspace/node	Network	
Raichu	64	2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz)	32 GB	400 GB	GbE	
Delcatty	160	2 x 8-core Intel E5-2670 (Sandy Bridge @ 2.6 GHz)	64 GB	400 GB	FDR InfiniBand	
Phanpy	16	2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz)	512 GB	3x 400 GB (SSD, striped)	FDR InfiniBand	
Golett	200	2 x 12-core Intel E5-2680v3 (Haswell-EP @ 2.5 GHz)	64 GB	500 GB	FDR-10 InfiniBand	
Swalot	128	2 x 10-core Intel E5-2660v3 (Haswell-EP @ 2.6 GHz)	128 GB	1 TB	FDR InfiniBand	2016-Q3

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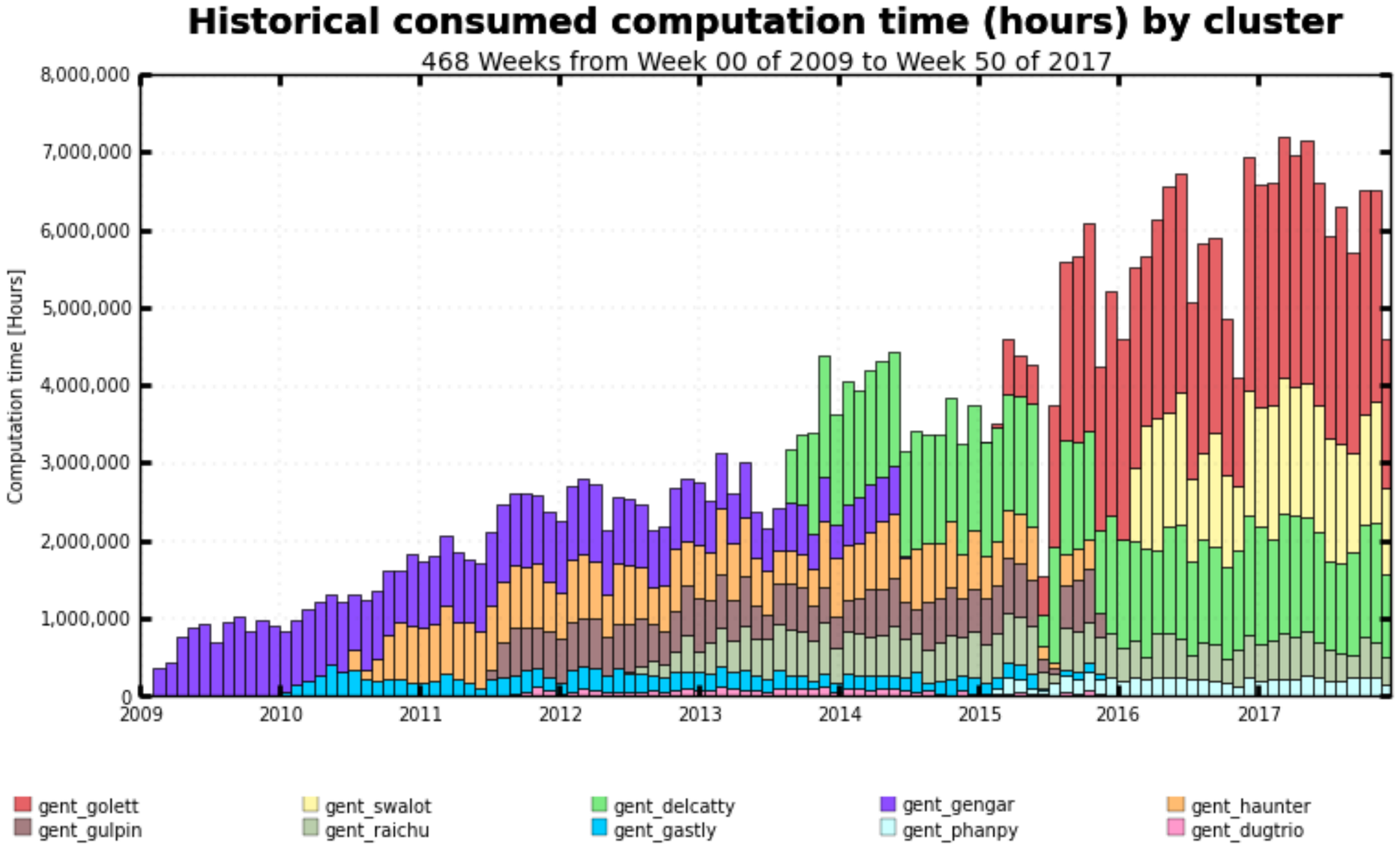
OVERVIEW OF HPC-UGENT USAGE



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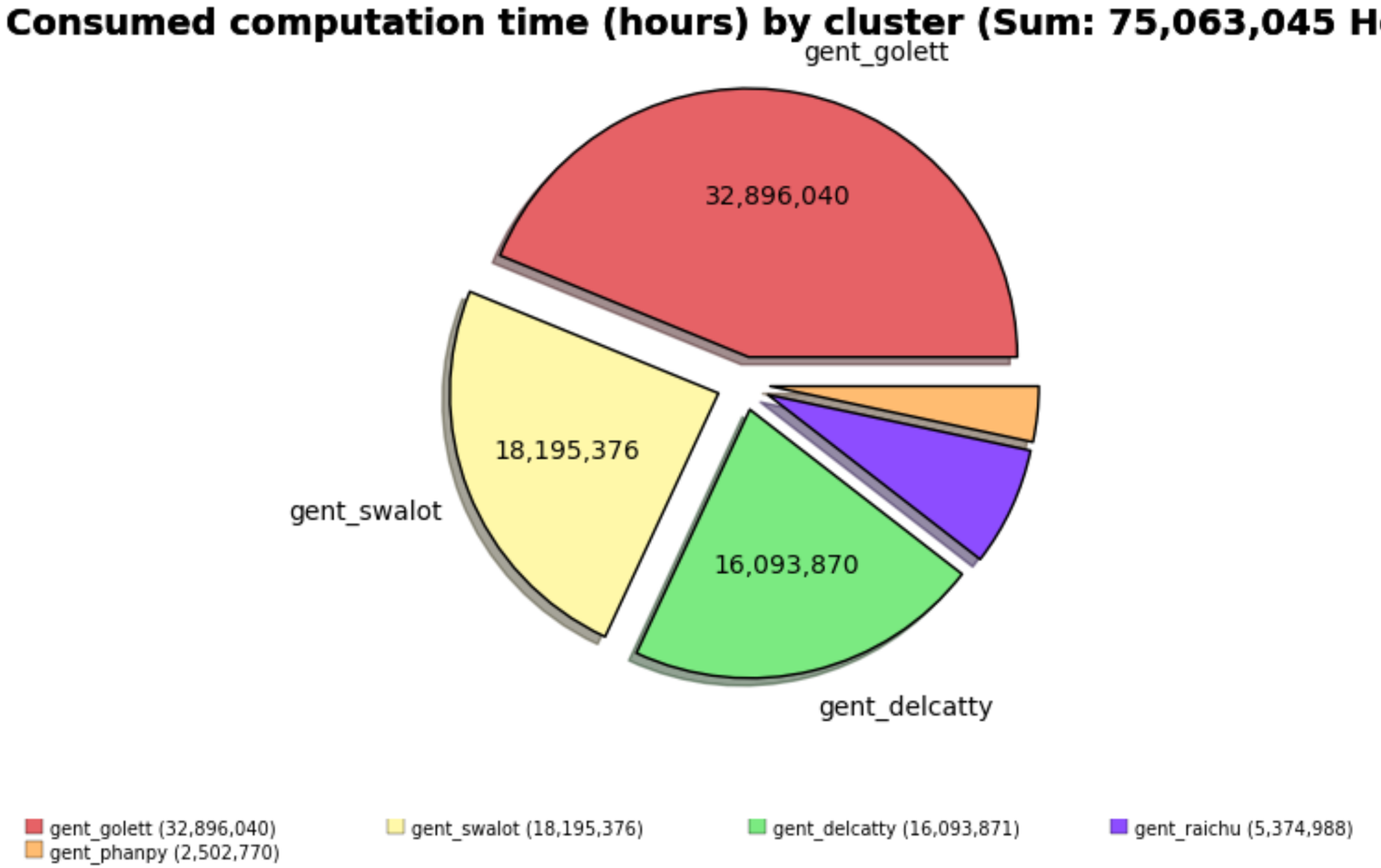
OVERVIEW OF HPC-UGENT USAGE



Consumed compute time in 2017		
	core years	use %
delcatty	1837	80%
phanpy	286	78%
raichu	614	72%
golett	3755	84%
swalot	2077	85%
	8569	82%

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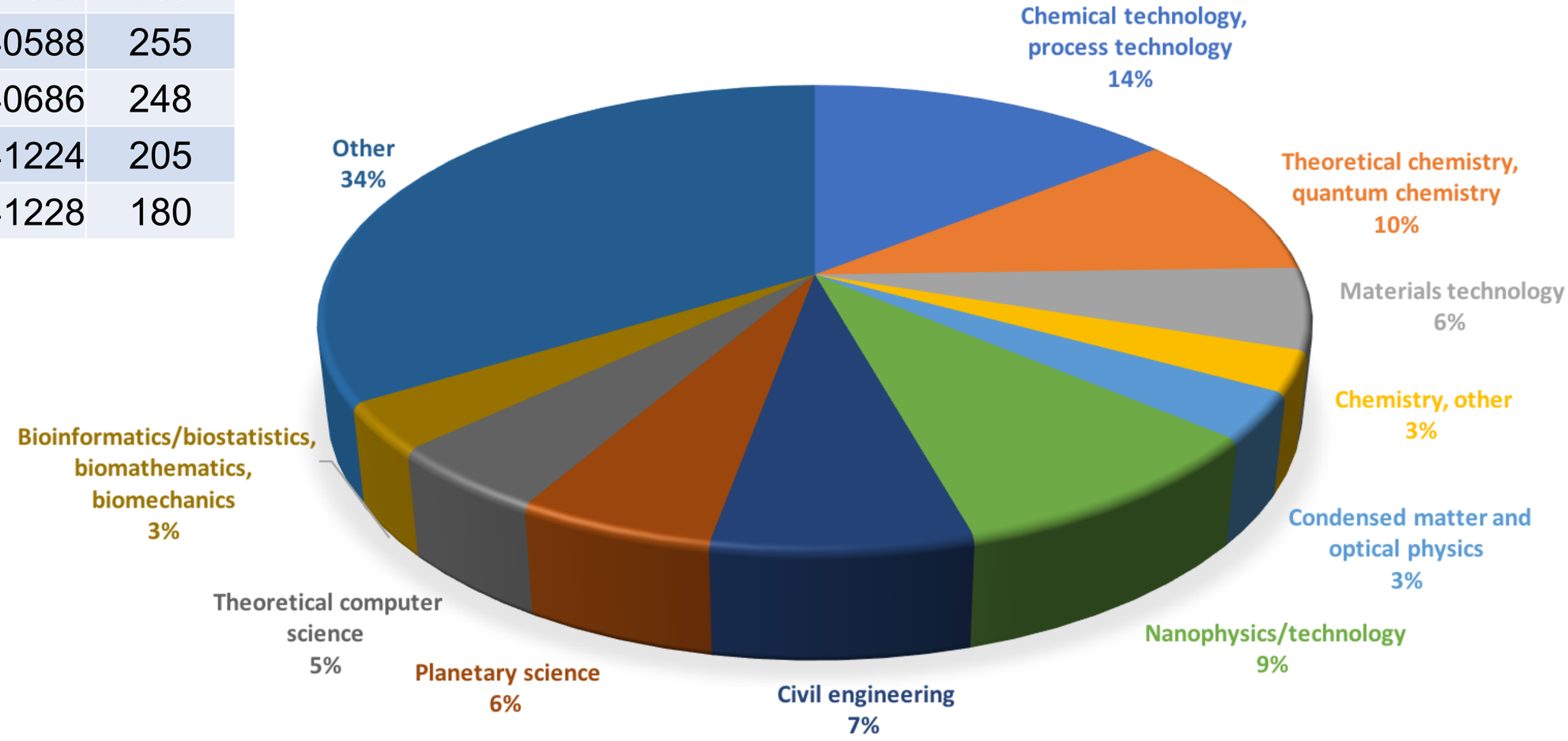
OVERVIEW OF HPC-UGENT USAGE

Top 10 users			
	core years		core years
vsc40941	477	vsc41326	285
vsc40944	473	vsc40588	255
vsc40484	470	vsc40686	248
vsc40309	398	vsc41224	205
vsc41948	301	vsc41228	180



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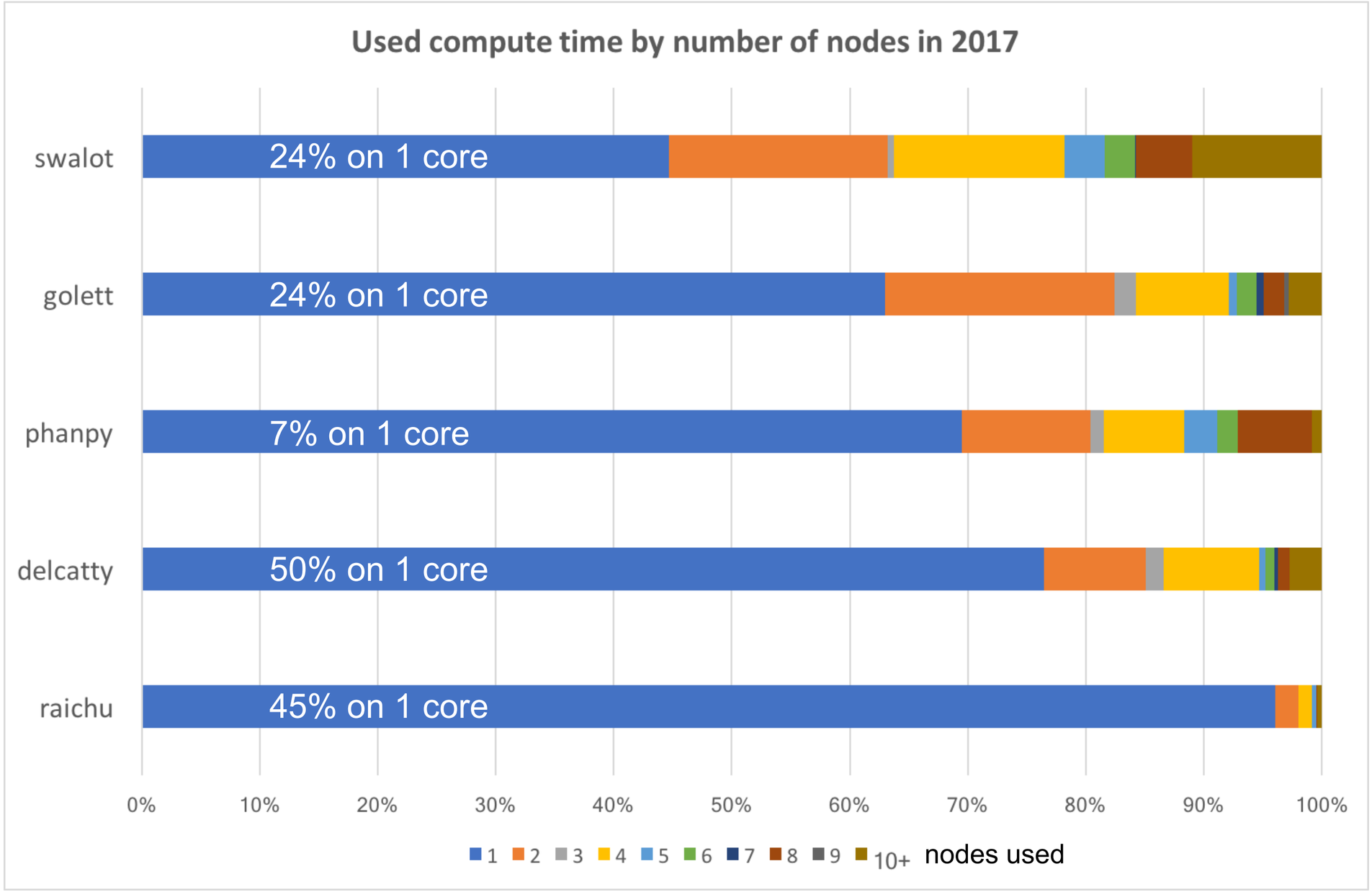
OVERVIEW OF HPC-UGENT USAGE



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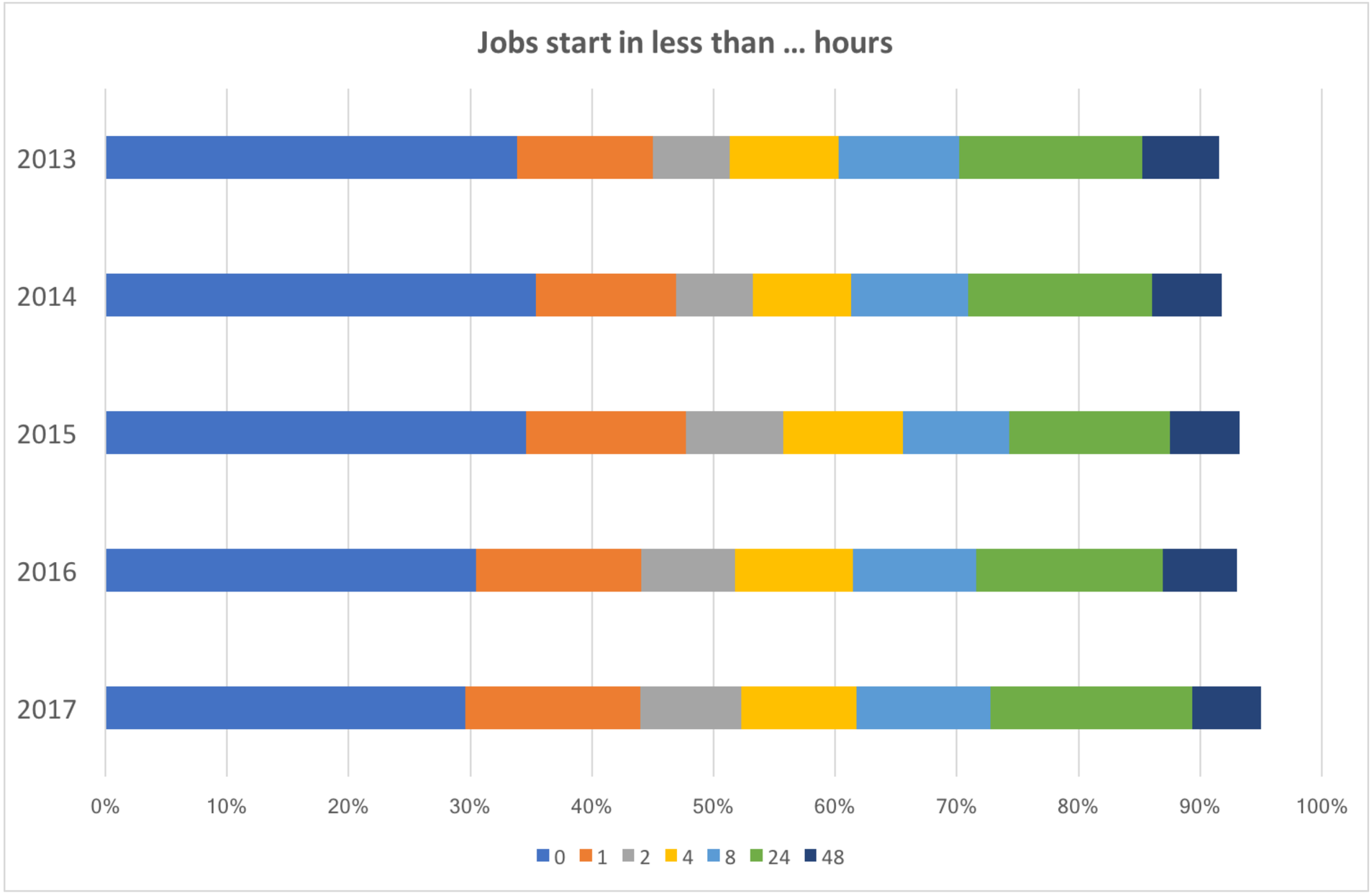
OVERVIEW OF HPC-UGENT USAGE



Total #jobs

2.842.286

4.108.474

4.098.513

3.186.564

4.785.543

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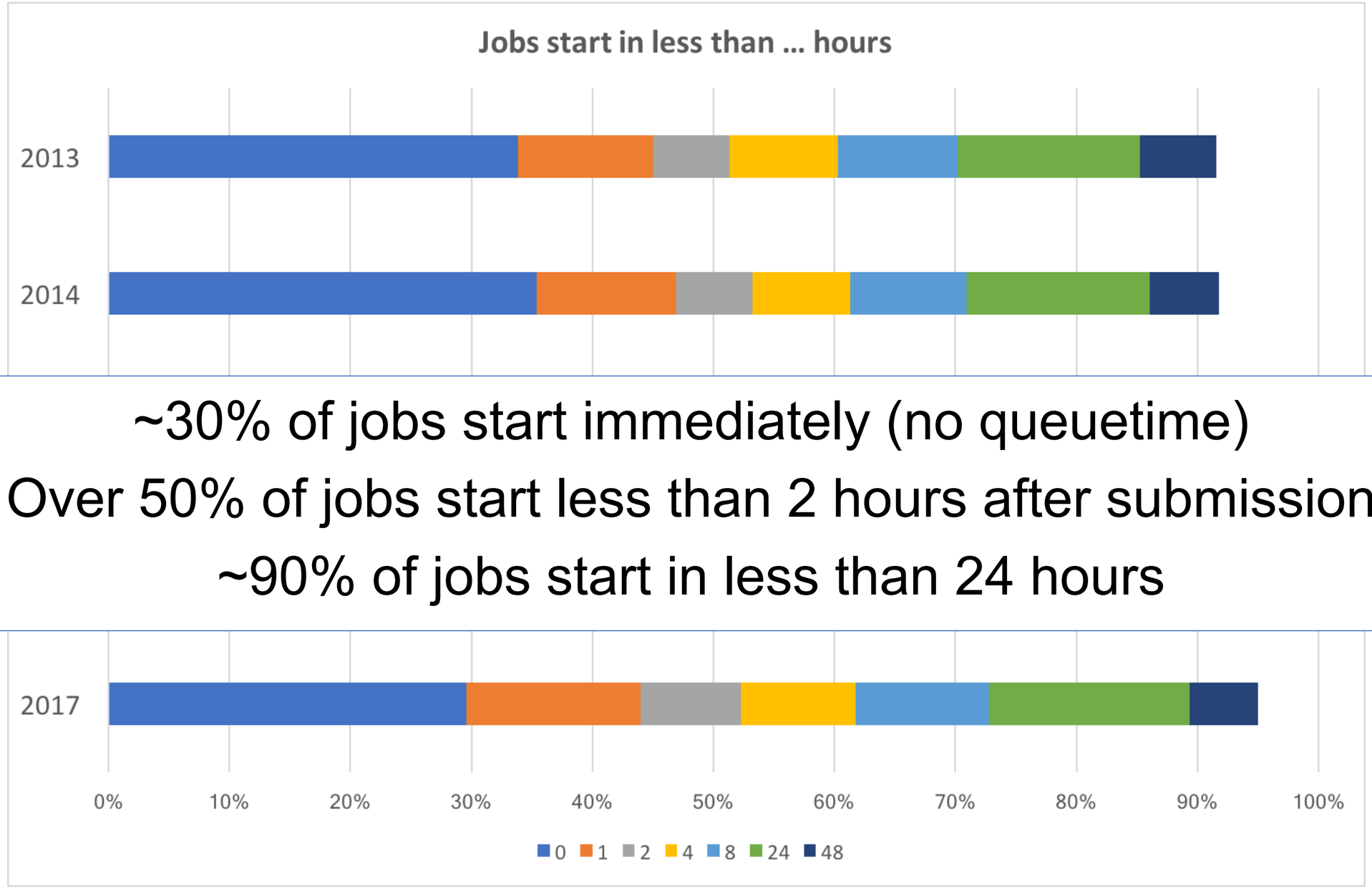
OVERVIEW OF HPC-UGENT USAGE



Total #jobs

2.842.286

4.108.474

~30% of jobs start immediately (no queuetime)

Over 50% of jobs start less than 2 hours after submission

~90% of jobs start in less than 24 hours

4.098.513

3.186.564

4.785.543

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HPC-UGENT – NEW SERVICES

Extra compute clusters

- 2.2M euro investment
- Production expected by summer 2018

#nodes	CPU	Mem/node	Disk/node	Network
72	2 x 18-core Intel Xeon Gold 6140 (**Skylake** @ 2.3 GHz) 2592 cores in total	192 GB	1 TB 240 GB SSD	EDR InfiniBand
96	2 x 18-core Intel Xeon Gold 6140 (**Skylake** @ 2.3 GHz) 3456 cores in total	96 GB	1 TB 240 GB SSD	10 GbE

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HPC-UGENT – NEW SERVICES

Extra compute clusters

- 2.2M euro investment
- Production expected by summer 2018

	#nodes	CPU	Mem/node	Disk/node	Network
 **skitty**	72	2 x 18-core Intel Xeon Gold 6140 (**Skylake** @ 2.3 GHz) 2592 cores in total	192 GB	1 TB 240 GB SSD	EDR InfiniBand
 **victini**	96	2 x 18-core Intel Xeon Gold 6140 (**Skylake** @ 2.3 GHz) 3456 cores in total	96 GB	1 TB 240 GB SSD	10 GbE

These clusters will replace delcatty and raichu

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HPC-UGENT – NEW SERVICES

Cloud testbed ‘grimer’

- 16 hypervisors - 256 CPU cores – 200 TB storage (Ceph)
- Reuse of decommissioned muk (old Tier-1) hardware
- For users with specific requirements
  - Public cloud infrastructure
  - Graphical user interface
  - Software with wallclock > 72h ? (But checkpointing is far more advisable)
- VM(s) managed by user! Currently free of charge
- Testbed to gather expertise – underlying technology may change

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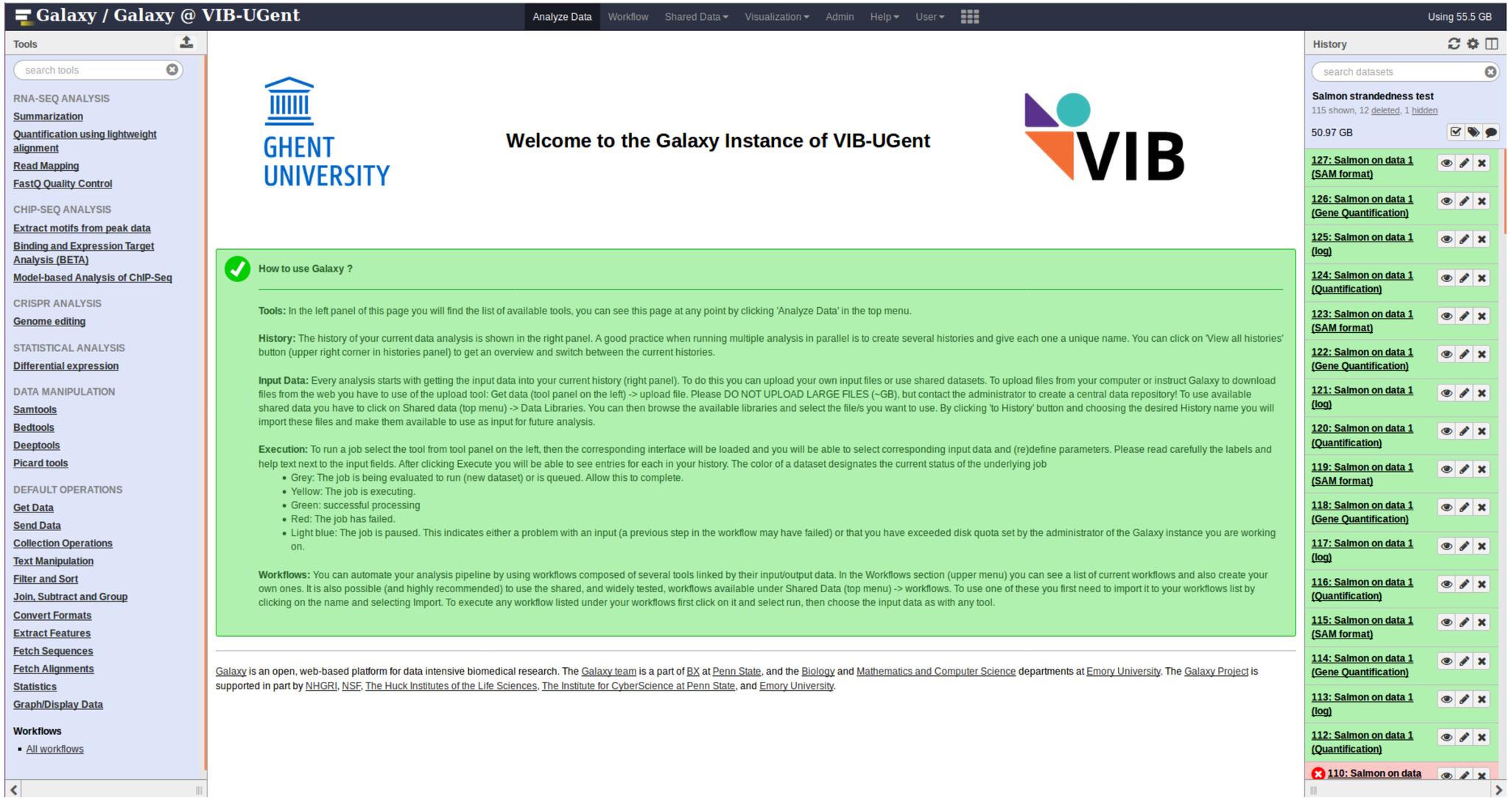
Contact hpc@ugent.be if you would like to be pilot

HPC-UGENT – NEW SERVICES

Cloud testbed ‘grimer’: example application



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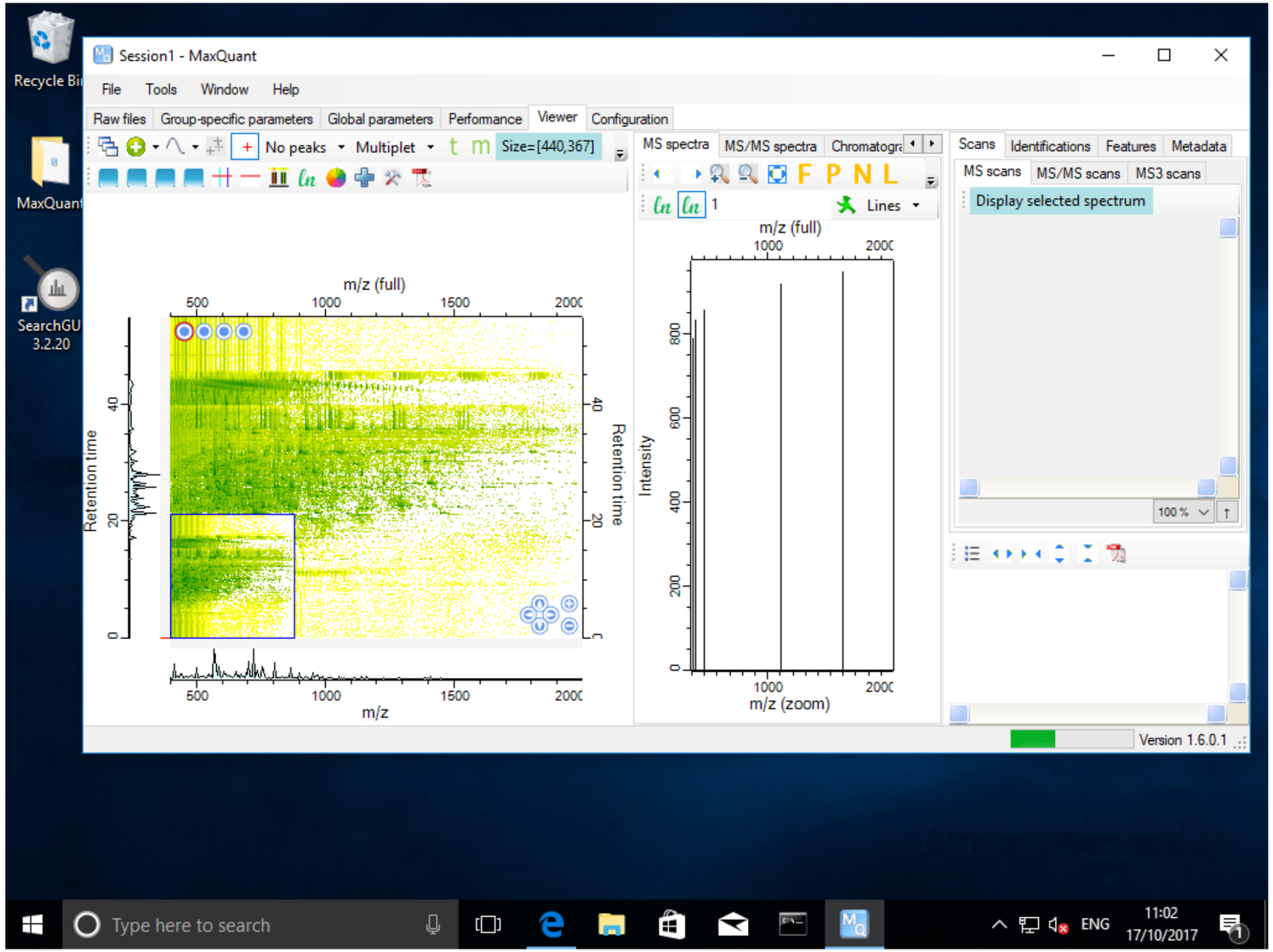
HPC-UGENT – NEW SERVICES

Cloud testbed ‘grimer’: example application



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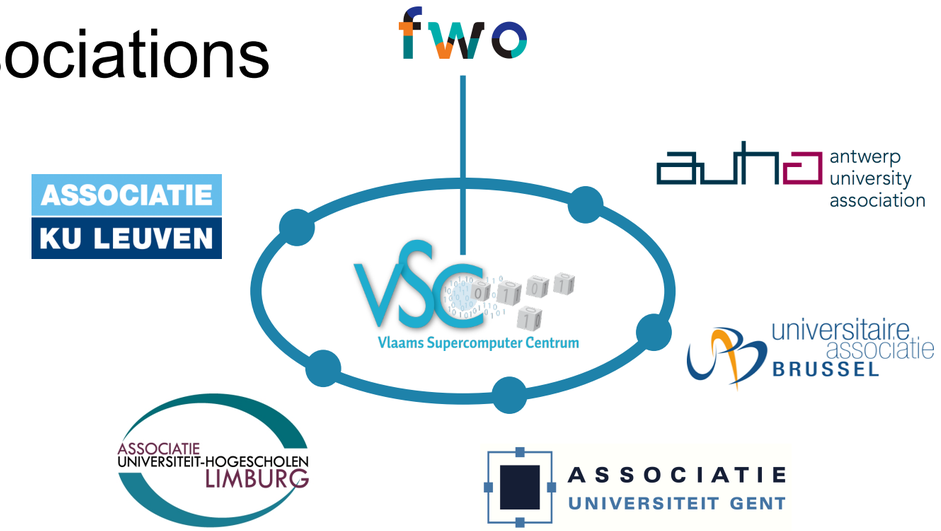
ABOUT VSC

VSC – Flemish Supercomputer Center

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



Mission

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

ABOUT VSC – GOVERNING BODIES

VSC steering group

- Daily (monthly) management of VSC, consensus
- UGent representative: Ewald Pauwels

Users committee

- Map user needs, advise on Tier1/2 operation, VSC user day
- UGent representatives: Veronique Van Speybroeck, Marie-Françoise Reyniers

Tier1 evaluation committee (non-Flemish experts)

- Technical evaluation of Tier-1 applications

Industrial board

- Advise to increase involvement of industry

FWO

- Funding, final governance

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ABOUT VSC - GOALS

1. Offer its target audience **access to diversified ICT infrastructure** that is tailored to the needs of scientific/technical computing.
2. Provide a **common user environment** on the computing infrastructure, which is available in the local hubs.
3. **Support** its users so that they can lift their research and development to a higher level by using scientific/technical computing.
4. **Inform about the capabilities and achievements** of scientific/technical computing and its potential added value.
5. Actively **promote scientific/technical computing in Flemish industry** and foster the exchange of ideas and expertise between research institutions and industry.
6. Offer a diverse and coordinated **training program** across the VSC consortium to stimulate and advance the uptake of scientific/technical computing in new and existing users.
7. Engage and actively participate in **international initiatives** such as PRACE and Horizon 2020, and cooperate with other centers focusing on scientific/technical computing.

VSC INFRASTRUCTURE

https://www.vscentrum.be/infrastructure/hardware

Available hardware

Tier-1

- Our current Tier-1 system is BrENIAC, operated by KU Leuven. The system is aimed at large parallel computing jobs that require a high-bandwidth low-latency interconnect. Compute time is again only available upon approval of a project. See the page on Tier-1 project access and links in that page.
- Our first Tier-1 system is muk, was operated by UGent but is no longer in production.

Experimental setup

- There is a small GPU and Xeon Phi test system which is can be used by all VSC members on request (though a project approval is not required at the moment). The documentation for this system is under development.

Free of charge

→ http://hpc.ugent.be/userwiki/index.php/Tips:Software:GPGPU

Tier-2

Four university-level cluster groups are also embedded in the VSC and partly funded from VSC budgets:

- The UAntwerpen clusters (hopper and leibniz)
- The VUB cluster (hydra)
- The UGent local clusters

Free of charge

- The KU Leuven/UHasselt cluster (ThinKing and Cerebro)

Not free of charge, but heavily discounted

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VSC INFRASTRUCTURE

Using other VSC infrastructure

- Don’t hesitate
- If unsure about pricing, ask KULeuven for quote

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

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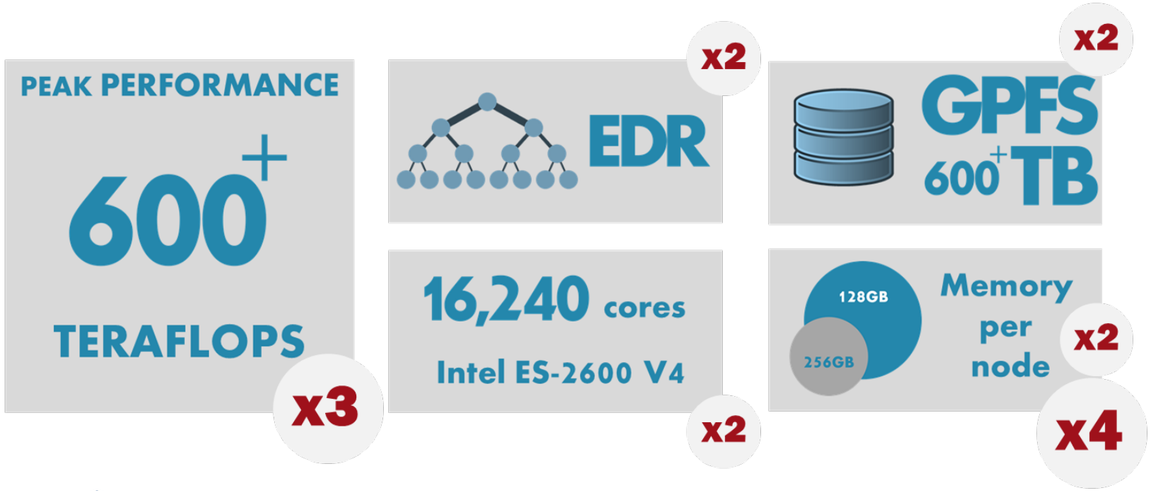
VSC INFRASTRUCTURE – TIER-1

Muk @ UGent → BrENIAC @ KULeuven



- 580 nodes
- 2 Intel Xeon Broadwell → 16.240 cores
- 128/256 GB RAM
- InfiniBand EDR interconnect
- 634 TB storage

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TIER-1 ACCESS – STARTING GRANT

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

- Purpose = explore, do scaling tests of your software, prepare for project
- 100 node days (= 100 x 28 x 24 = 67.200 core hours)
- Available for 2 months
- Personal grant
- Fast submission procedure, very short proposal
- Constantly reviewed
- Success rate = 100%

- FREE OF CHARGE

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TIER-1 ACCESS – PROJECT ACCESS

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

- 500 - 5000 node days (= 336.000 – 3.360.000 core hours)
- Available for 6 months
- Can be granted to multiple researchers
- Reviewed 3x per year by Tier-1 Evaluation Committee
  - Next deadline = 5 February 2018
- Success depends on quality of your proposal
  - Send your proposal to hpc@ugent.be for prior review

- FREE OF CHARGE

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VSC INFRASTRUCTURE TIER-1

BrENIAC: A year celebrating curiosity

3 calls

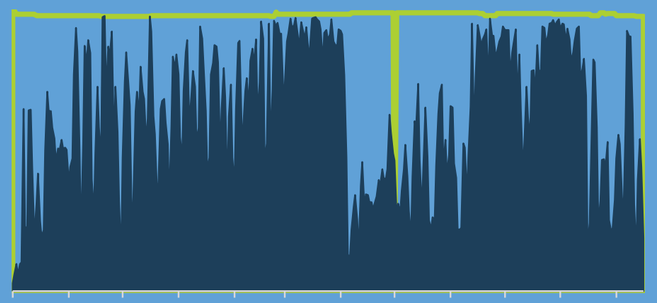
81 users

59 projects

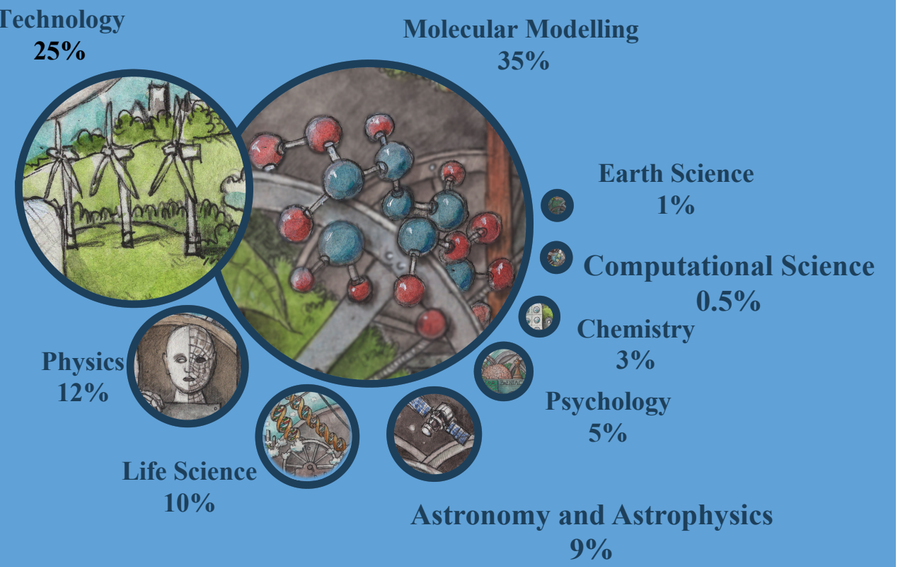
72,000 jobs

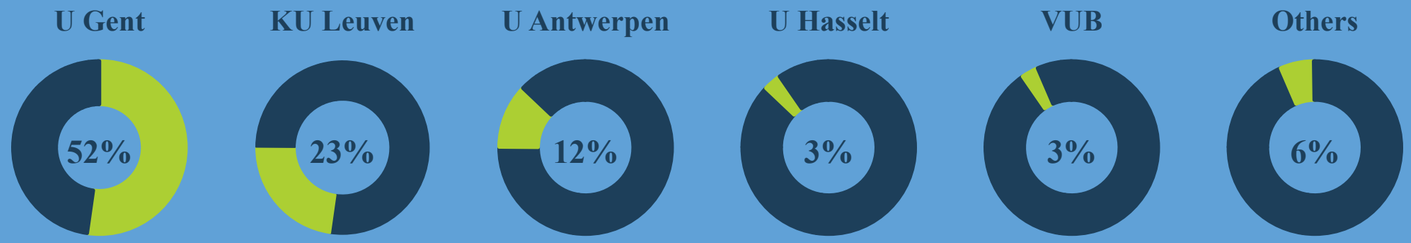
87M core hours

98% uptime



61% usage





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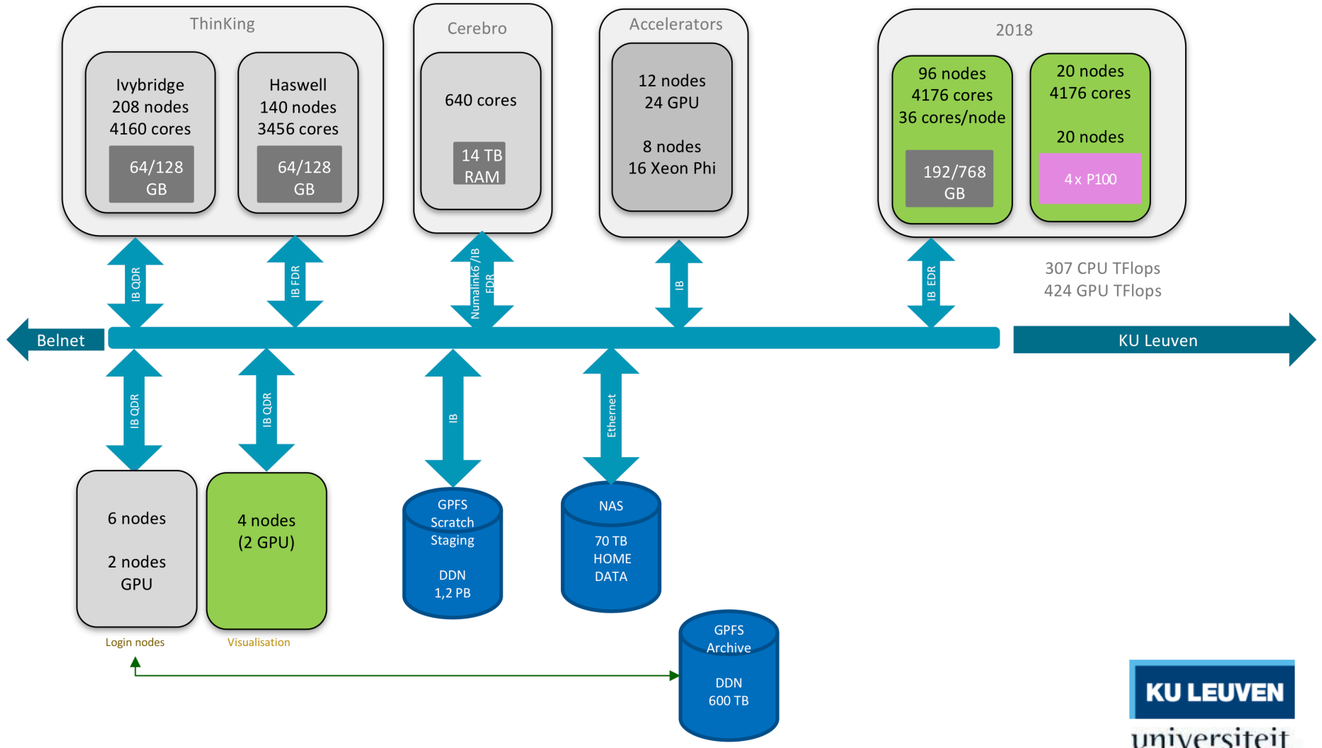
VSC - FUTURE PLANS

New GPU cluster at KULeuven



- 20 nodes with each
  4 x Nvidia Tesla P100

- KULeuven will likely open (free) pilot access to GPUs
- Let us know via hpc@ugent.be if you would like to use these GPUs

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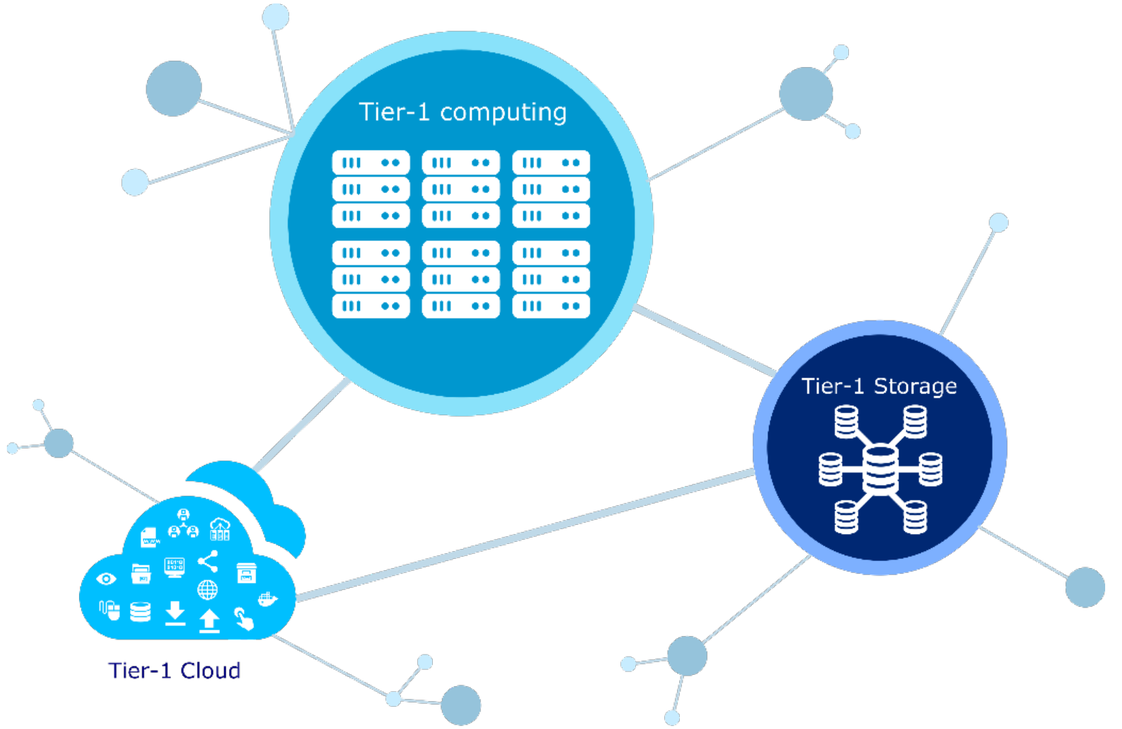
VSC - FUTURE PLANS

New Tier-1 supercomputing platform

(Subject to final approval by government)



- Intention to be structural
- Complementary programs
  - Cloud
  - Storage

  } very challenging
  - Compute: extending current Tier-1 service

- First developments proposed starting 2018

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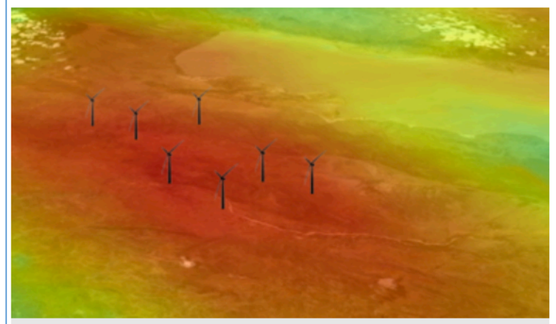
VSC – CALL FOR SUCCESS STORIES

Cases and projects

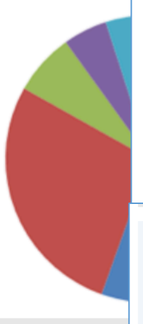
Achievements on our infrastructure

Industrial use cases



Wind energy simulations at 3E NV

3E NV, a Belgian renewable energy consultancy firm, makes use of the VSC infrastructure and



Janssen P

Janssen Pha
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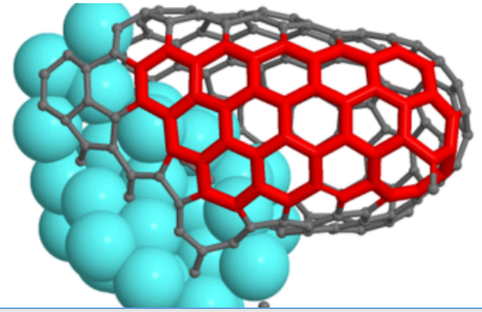
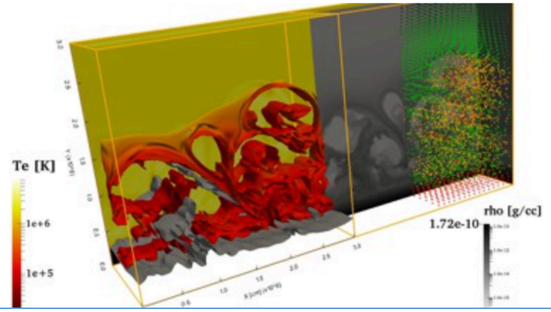
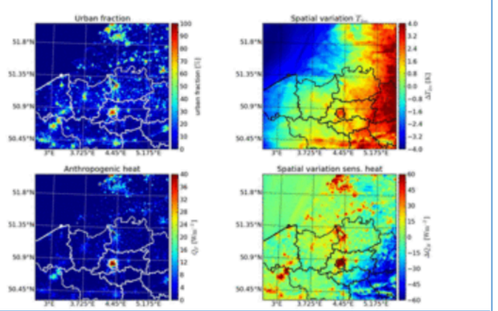
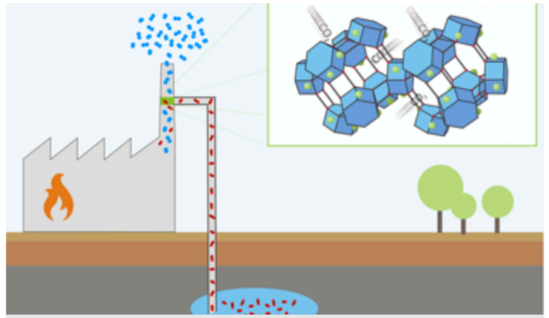
Academic use cases

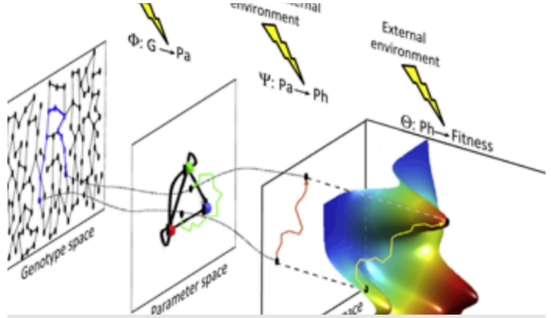




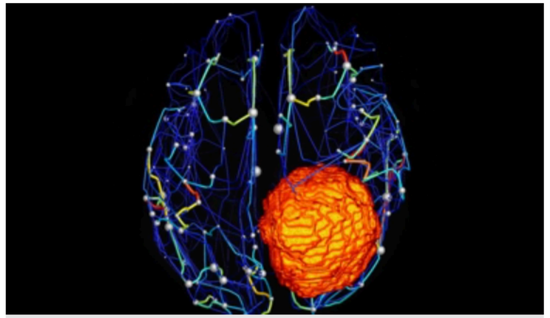




Molecular modeling spurs innovative technology against global warming



Mechanistic modeling and in silico evolution of gene regulatory networks



Modeling brain dynamics in health and disease using supercomputing

Prof. Daniele Marinazzo (UGent) uses

https://www.vscentrum.be/en/project-and-cases

Contact hpc@ugent.be if you could contribute

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REVIEW OF USER POLL RESULTS

- 104 respondents
- ~8 questions
- Average completion time: 5 minutes

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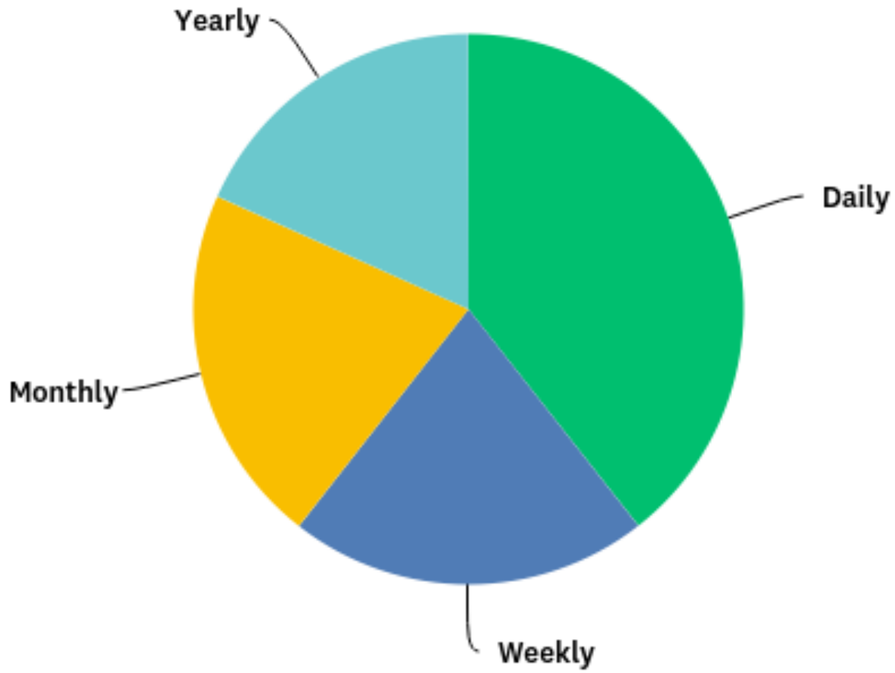
REVIEW OF USER POLL RESULTS

How often do you use the HPC-UGent scientific computing infrastructure?

	#resp
On a daily basis	41
Usually once per week	22
Once per month	22
1-2 times per year or less	19



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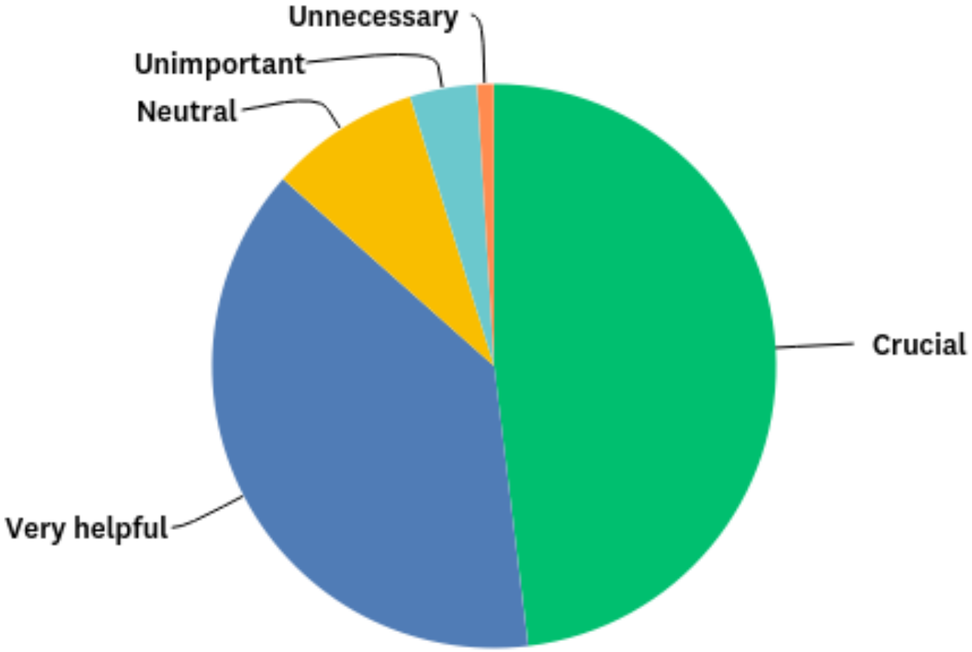
REVIEW OF USER POLL RESULTS

How important is HPC-UGent for your research?

	#resp
Crucial.	50
I can't do my research without.	
Very helpful.	40
It allows me to do my research at a faster pace and at a higher level.	
Neutral	9
Unimportant.	4
I can just as well do my research in another way.	
Unnecessary.	1
I don't need it at all to do my research.	



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REVIEW OF USER POLL RESULTS

How often / How important?

How important for your research?	How often do you use?				
		Daily	Weekly	Monthly	Yearly
	Crucial	**32%**	7%	7%	3%
	Very helpful	7%	**14%**	**13%**	5%
	Neutral	1%	0%	2%	**6%**
	Unimportant	0%	0%	0%	**4%**
	Unneccesary	0%	0%	0%	**1%**

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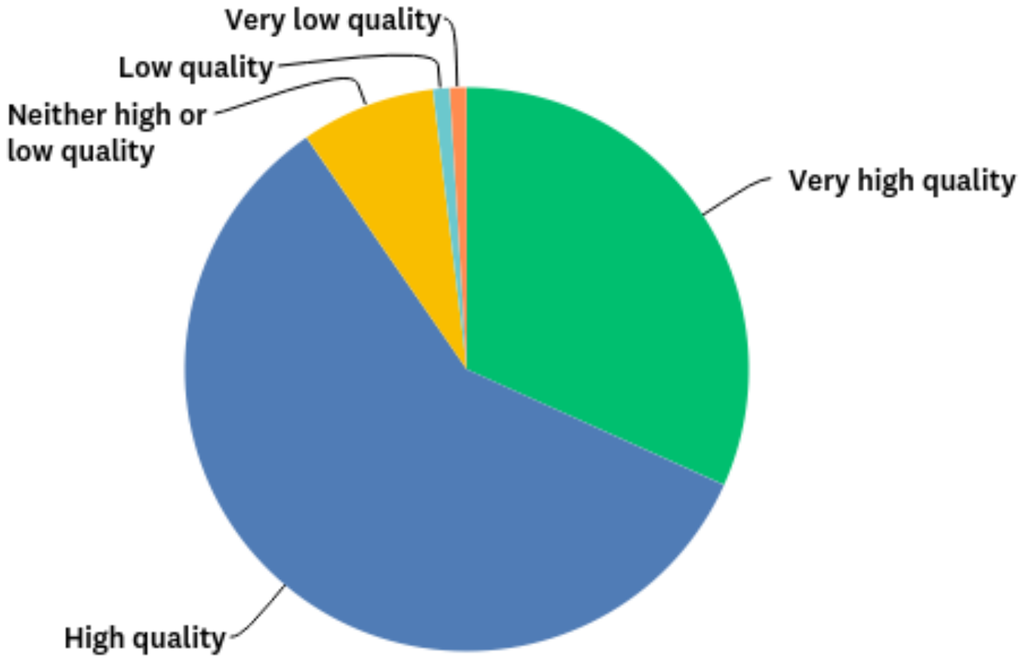
REVIEW OF USER POLL RESULTS

How would you rate the services that HPC-UGent provides?
(compute clusters, login nodes, training, user support, website)

	#resp
Very high quality	33
High quality	61
Neither high or low quality	8
Low quality	1
Very low quality	1



More than 90% of poll participants rate our services as ‘high quality’ or above.

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REVIEW OF USER POLL RESULTS

How often / Your rating?

	How often do you use?				
Your rating of our services?		Daily	Weekly	Monthly	Yearly
	Very high quality	**15%**	**8%**	**7%**	2%
	High quality	**21%**	**12%**	**13%**	**13%**
	Neither high or low quality	2%	2%	0%	4%
	Low quality	1%	0%	0%	0%
	Very low quality	0%	0%	1%	0%

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REVIEW OF USER POLL RESULTS

Is there a particular service that stands out or you care to comment about? ☺☺☺

#comments	Service	
16	User Support	*excellent, fast, friendly*
8	Training	*regular, hands-on*
6	Infrastructure	*diverse, reliable, updated*
5	Software	*fast installation, version flexibility, module system*
4	Documentation	*good, excellent, usable by newbies*

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REVIEW OF USER POLL RESULTS

Is there a particular service that stands out or you care to comment about? ☺☺☺

“The clusters in Ghent are still the best managed systems I've been working with. Keep up the nice work guys!”

”The Helpdesk is extremely supportive and helpful! Thank you!”

”The consistent use of the system status page in the User Portal of the VSC website is much appreciated. It is good to have this page as the single point of information for cluster related updates and during upsets.”

→ https://www.vscentrum.be/en/user-portal/system-status

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REVIEW OF USER POLL RESULTS

Is there a particular service that stands out or you care to comment about? ☹☹☹

#comments	Service	
5	Infrastructure	*long queues, wallclock, regular downtimes*
1	Training	*software-specific training sessions*
1	Documentation	*spread out, no overview of basic commands*

REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

- 62 responders
- 92 suggestions
- Detailed follow-up in future
- Recurring suggestions in next slides

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REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

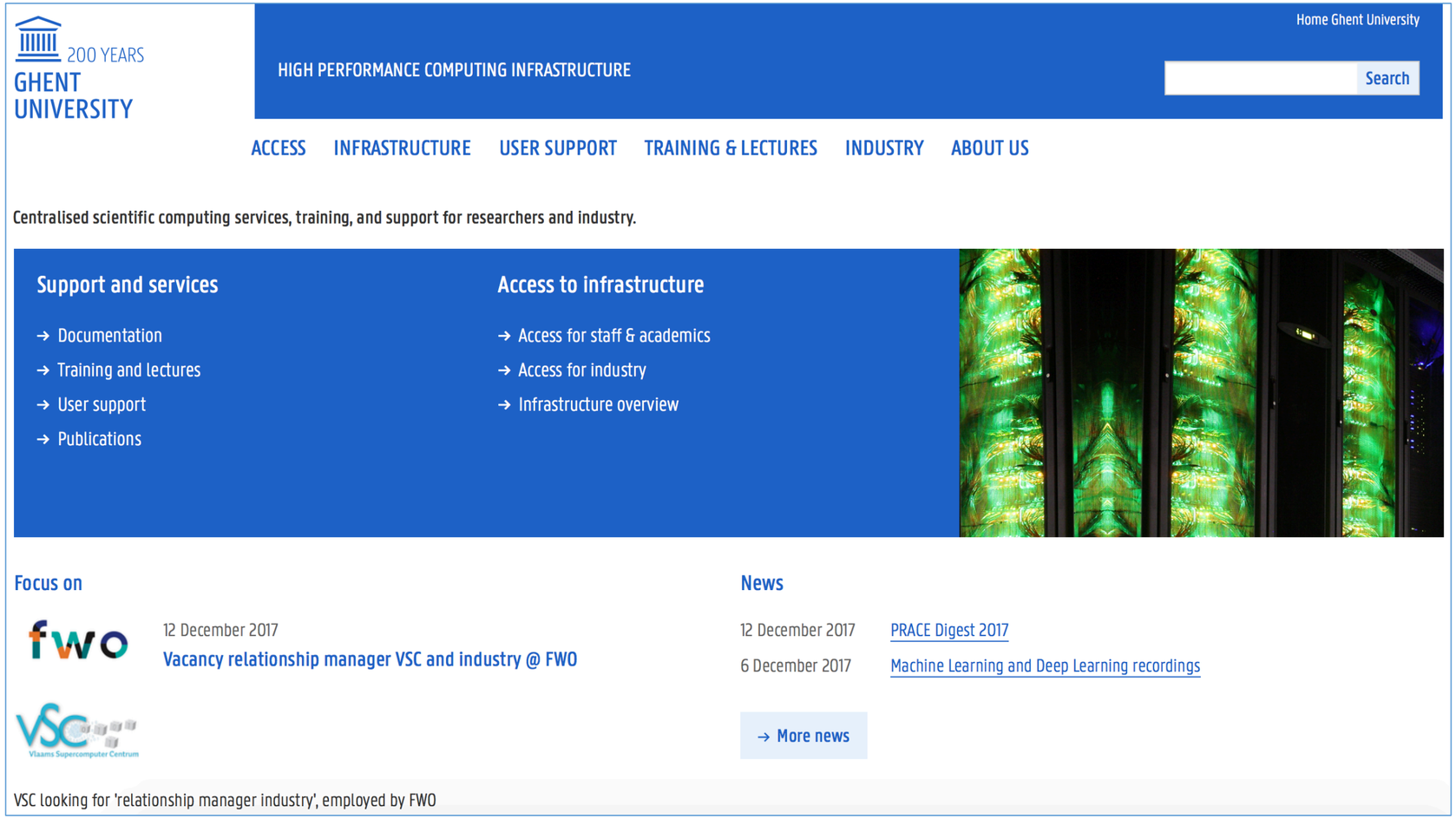
Documentation (21)

- More structured wiki/website that is SPOI (6)
- Documentation better geared towards new users (9)
  - Checklist for starters
  - Different clusters + storage locations
  - Frequently used commands
- More examples: scripts, software (3)
- Updated documentation (2)
- Newsletter

REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

Documentation (21)



REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

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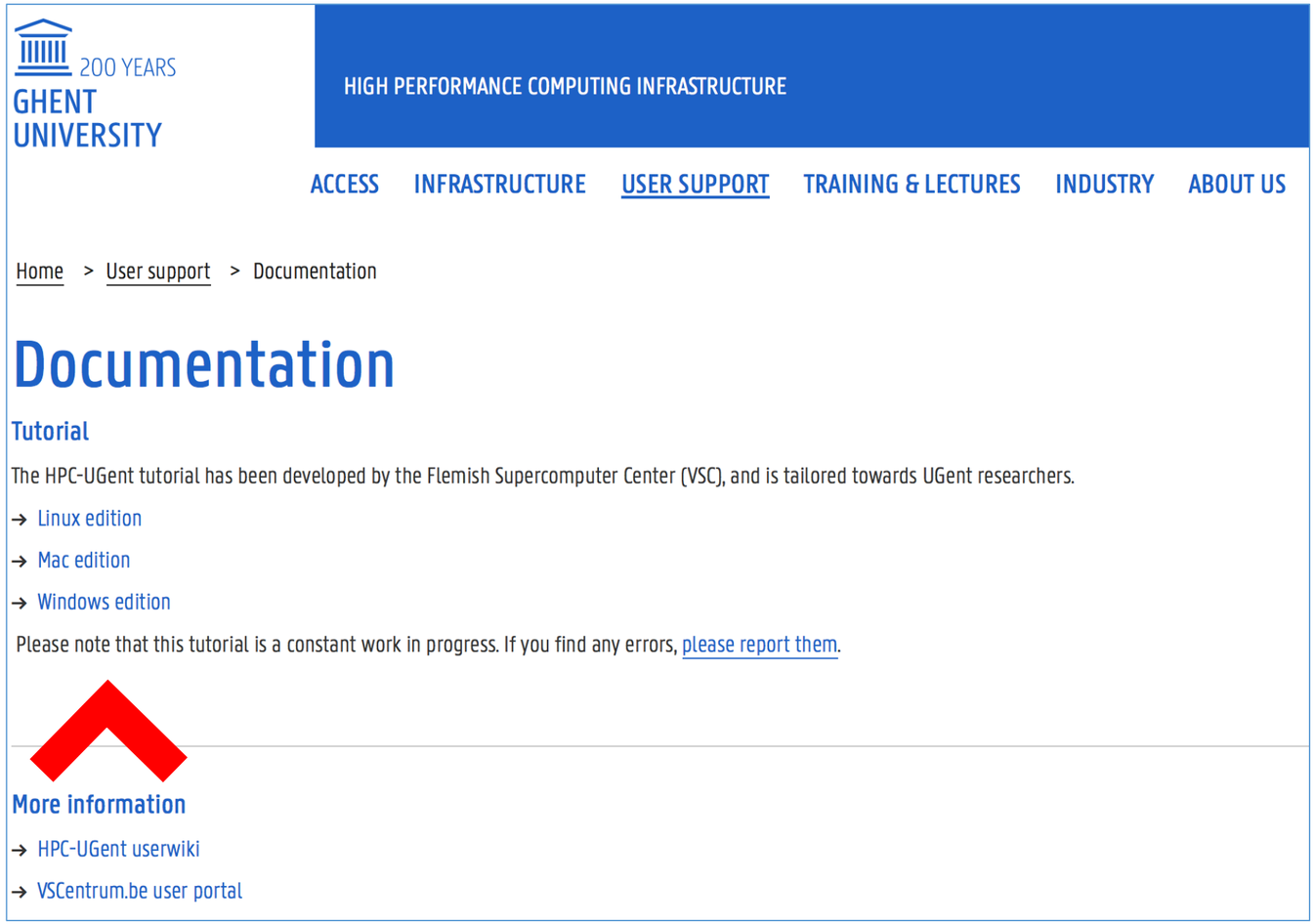

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REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

User experience (21)

- Shorter queue times (7)
- Way to estimate queue time (4)
- Longer wallclock time (4)
  - http://hpc.ugent.be/userwiki/index.php/User:Checkpointing
  - contact hpc@ugent.be if you have checkpointing issues
- Feedback on efficiency of specific job (4)

Infrastructure (17)

- Larger compute power (7)
- GPU (4)
- Debug infrastructure, remote visualization (2)

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REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

Data (10)

- More storage
- Easier sharing of data
  - Between VOs
    - VSC_DATA_SHARED in https://account.vscentrum.be/django/vo/edit
  - Public → VMs ?
- Staging in/out data
- Archive data of inactive users

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REVIEW OF USER POLL RESULTS

How could we further improve HPC-UGent services?

User support (3)

More HPC-UGent staff

Training (7)

More (5)

Policy (4)

Collaboration within VSC

Keep services free of charge

Security (6)

ftp connectivity (5) ?

Node sharing, data visible to other users

Software (3)

Form to request software install/update

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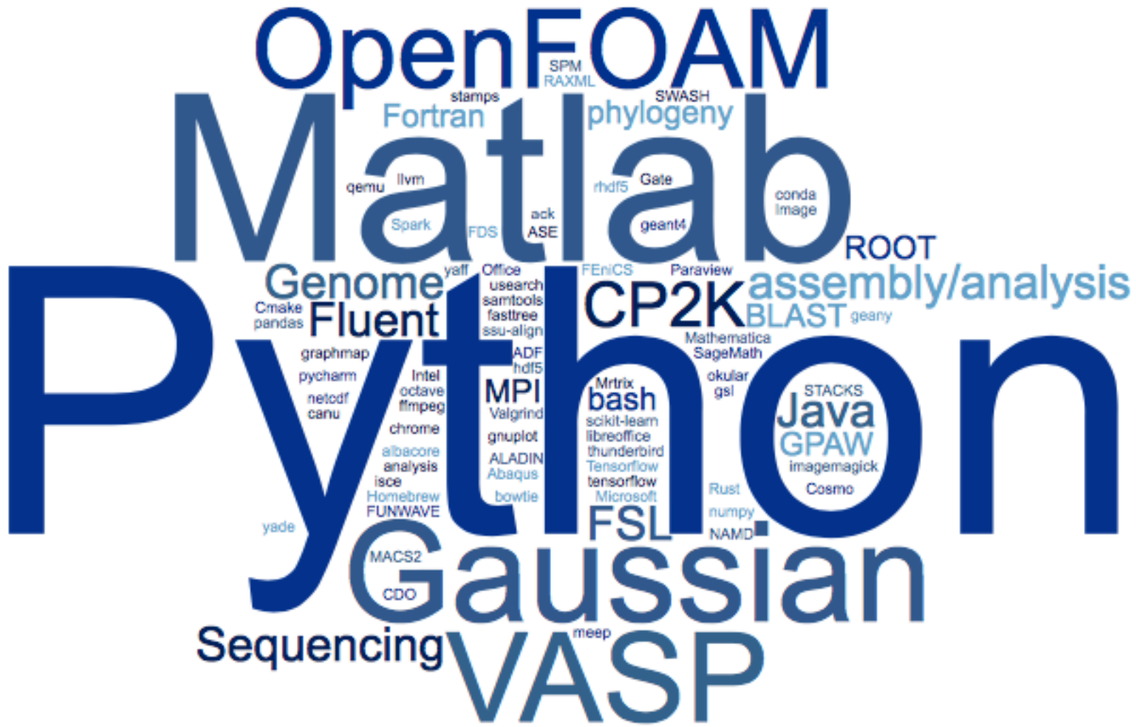
REVIEW OF USER POLL RESULTS

Which software do you typically use?

Python	24
Matlab	15
R	14
Gaussian	9
VASP	8
OpenFOAM	7
C, C++	7
CP2K	4
Own code	4
FSL	3
…	



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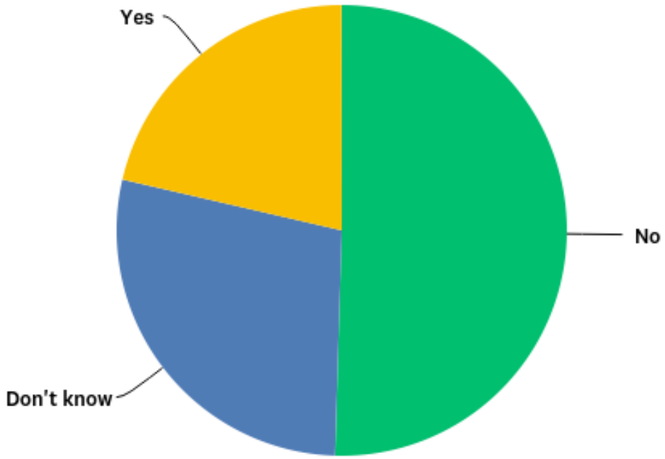
REVIEW OF USER POLL RESULTS

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

	#resp
No The current compute platform suffices	52
I don't know	29
Yes I need specific hardware/services	22



Specific hardware/services suggested

- Bigdata cluster with fast I/O
- Large, shared storage (many TB)
- Very high memory machine (1 TB)
- GPU
- More cores / node

- Other compilers than Intel
- Longer wallclock time
- Personnel to support coding design
- Additional personnel for software installs

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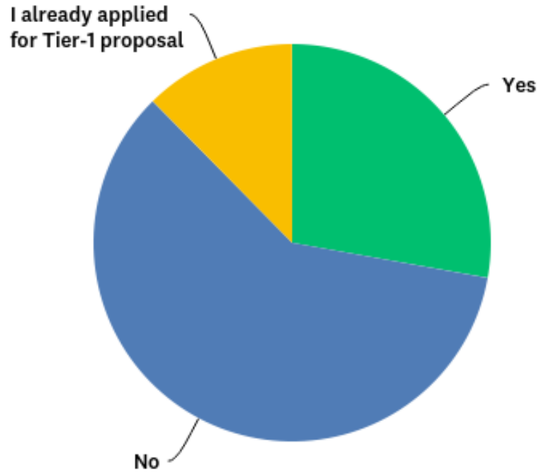
REVIEW OF USER POLL RESULTS

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

	#resp
Yes	27
I already applied for Tier-1 proposal	22
No	58



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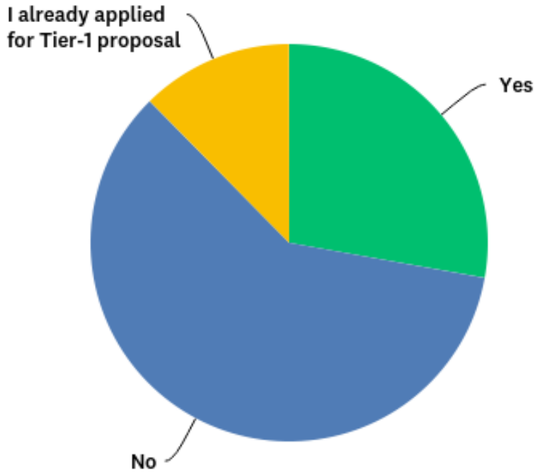

What is holding you back to submit a Tier-1 proposal?

Why do you consider Tier-1 not suitable for your research?

- Tier-2 suffices (33)
- Lack of experience (3)
- Don't know what Tier-1 is (3)
- Too much work (1)
- Gaussian does not scale (1)
- Additional cost (1)

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Vice-coordinator VSC

HPC-UGent

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RECEPTION: BEERS

Pils 13 Fresh Hop

The Ministry of Belgian Beers

Pils (4% Alc. Vol)

Zwaluw

Siphon Brewing

Session IPA (3,3% Alc. Vol)

Cendre

Siphon Brewing

Black saison (6.5% Alc. Vol)

Huldra

Brouwerij Totem

Session IPA (2,7% Alc. Vol)

Kornkråke Double Dry Hopped

Brouwerij Totem

Chili IPA (5,3% Alc. Vol)

Narvi

Brouwerij Totem

Mandarine Radler (2,1% Alc. Vol)

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