HPC - introduction

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ICTS, Leuven

https://github.com/hpcleuven/HPC-intro

8 October 2019

What is HPC

High-performance computing (HPC) uses supercomputers and computer clusters to solve advanced computation problems.

What a supercomputer is **NOT**

Actually, it is more like …….

The concept is simple: **Parallelism** = applying multiple processors to a single problem

Why supercomputer?

- Consider your favorite computational application
  - One processor can give results in N hours
  - Why not use N processors
    -- and get the results in just one hour?
- The concept is simple: **Parallelism** = applying multiple processors to a single problem

Parallel Computing

- Serial:
  - one program, on one core
- ’Embarrassingly parallel’ problems:
  - lots of runs of one program, with different parameters
- Problems that require ’real’ parallel algorithms
  - OpenMP
  - MPI : Message Passing Interface

Talk to us about
worker framework

Lucky
you!

Overview

- What is the VSC?
- What is a cluster?
- Infrastructure
- Software environment
- How to get started
- How to submit jobs
- Hands-on

VSC
& compute clusters

Vlaams Supercomputer Centrum (VSC)

- VSC is a virtual organization, founded in 2007
  - Goals
    - Provide infrastructure for high performance computing
    - Provide support for high performance computing
  - Participants: Flemish universities & associations
  - Funding
    - FWO/Hercules Foundation
    - Flemish government (EWI)
  - Virtual
    - But with real hardware
    - 1 user database
    - Uniform user experience

HPC services

Basic support

- Monitoring and reporting
- Helpdesk (hpcinfo@kuleuven.be)

Application support

- Installation and porting
- Optimisation and debugging
- Benchmarking
- Workflows and best practices

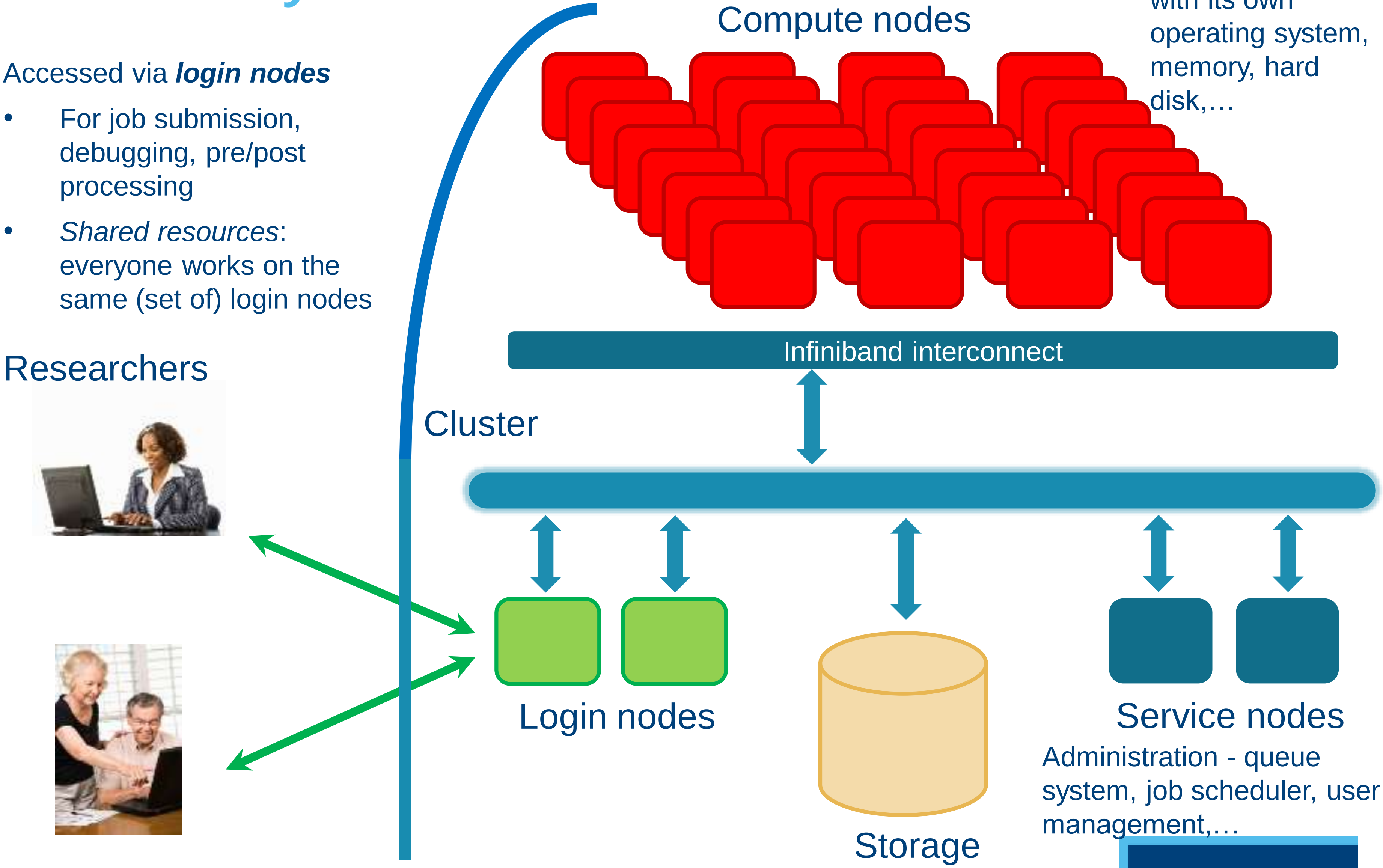
Training

- Documentation and tutorials
- Scheduled trainings / workshops
- On request workshops
- One-to-one sessions

Bird's eye view on a cluster

Accessed via ***login nodes***

- For job submission, debugging, pre/post processing
- *Shared resources*: everyone works on the same (set of) login nodes



Researchers

Cluster

Compute nodes

Many independent computers, each with its own operating system, memory, hard disk,…

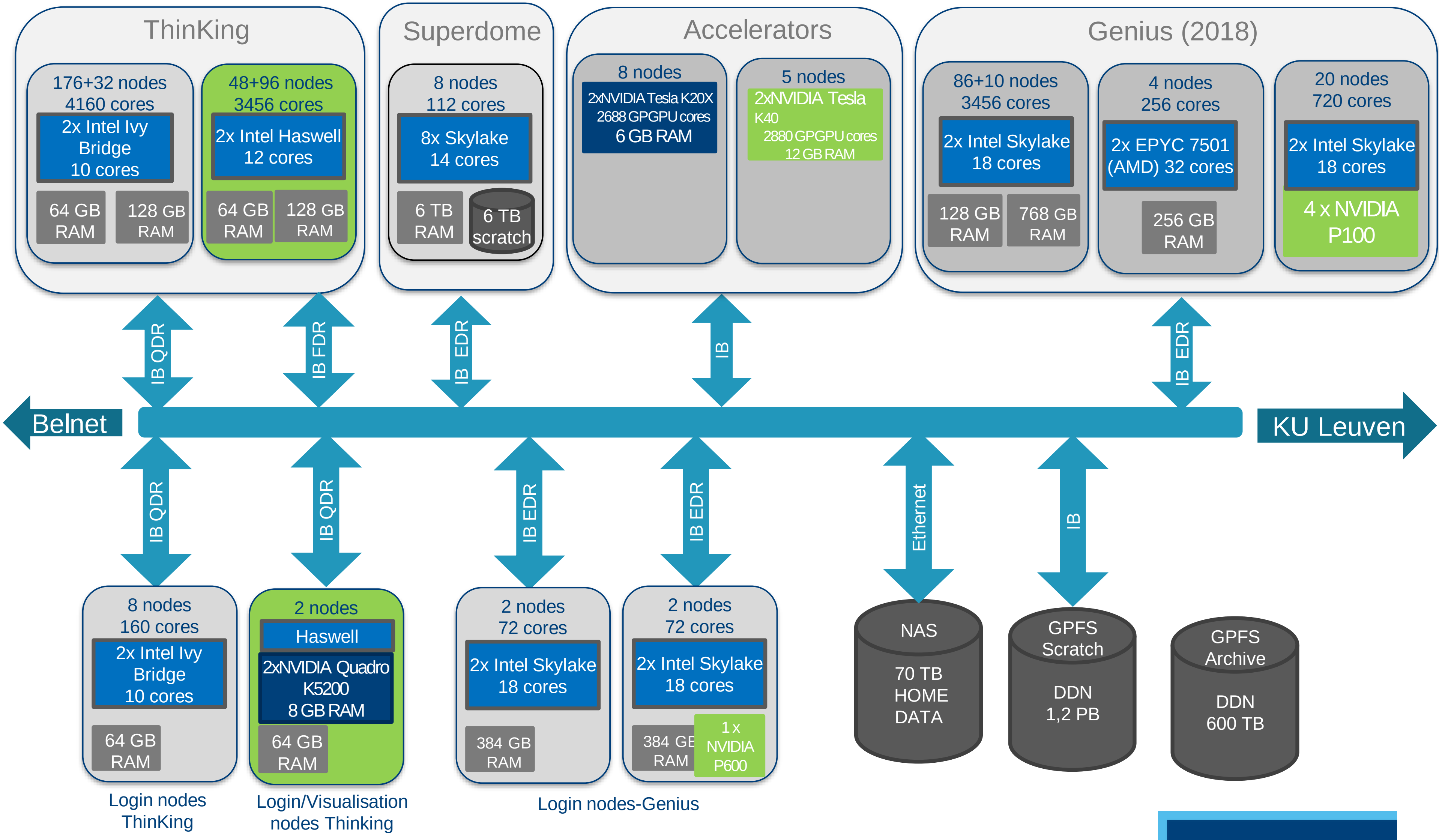
Infiniband interconnect

Login nodes

Storage

Service nodes

Administration - queue system, job scheduler, user management,…



ThinKing

176+32 nodes
4160 cores
2x Intel Ivy Bridge
10 cores
64 GB RAM
128 GB RAM

48+96 nodes
3456 cores
2x Intel Haswell
12 cores
64 GB RAM
128 GB RAM

Superdome

8 nodes
112 cores
8x Skylake
14 cores
6 TB RAM
6 TB scratch

Accelerators

8 nodes
2xNVIDIA Tesla K20X
2688 GPGPU cores
6 GB RAM

5 nodes
2xNVIDIA Tesla K40
2880 GPGPU cores
12 GB RAM

Genius (2018)

86+10 nodes
3456 cores
2x Intel Skylake
18 cores
128 GB RAM
768 GB RAM

4 nodes
256 cores
2x EPYC 7501 (AMD) 32 cores
256 GB RAM

20 nodes
720 cores
2x Intel Skylake
18 cores
4 x NVIDIA P100

IB QDR
IB FDR
IB EDR
IB
IB EDR

Belnet

KU Leuven

IB QDR
IB QDR
IB EDR
IB EDR
Ethernet
IB

8 nodes
160 cores
2x Intel Ivy Bridge
10 cores
64 GB RAM

Login nodes ThinKing

2 nodes
Haswell
2xNVIDIA Quadro K5200
8 GB RAM
64 GB RAM

Login/Visualisation nodes Thinking

2 nodes
72 cores
2x Intel Skylake
18 cores
384 GB RAM

2 nodes
72 cores
2x Intel Skylake
18 cores
384 GB RAM
1 x NVIDIA P600

Login nodes-Genius

NAS
70 TB HOME DATA

GPFS Scratch
DDN
1,2 PB

GPFS Archive
DDN
600 TB

KU LEUVEN

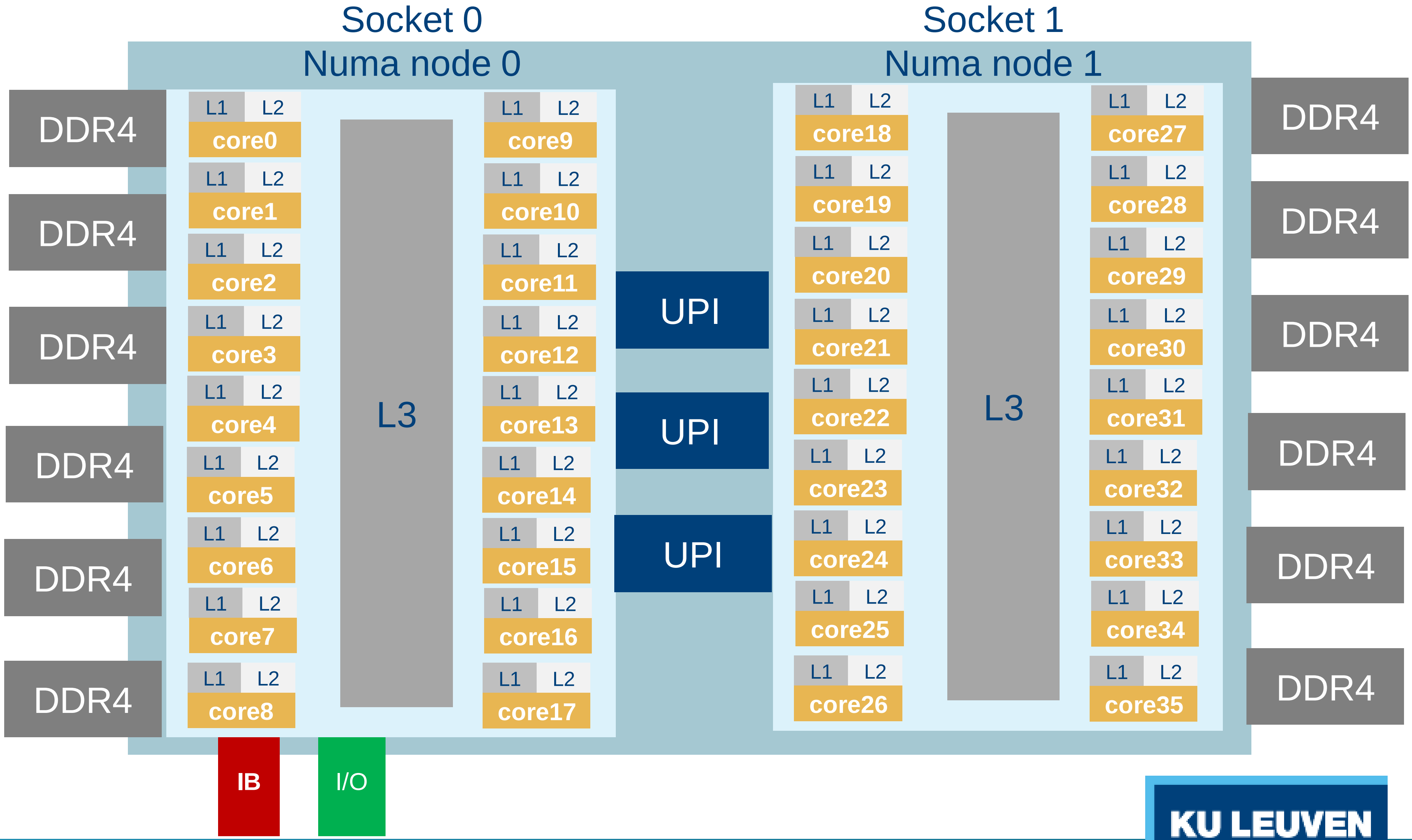
Genius

New cluster

Genius (2018)

Type of node	CPU type	Inter-connect	# cores	installed mem	local discs	# nodes
SkyLake	Xeon 6140	IB-EDR	36	192 GB	800 GB	86
SkyLake large mem	Xeon 6140	IB-EDR	36	768 GB	800 GB	10
SkyLake GPU	Xeon 6140 4xP100 SXM2	IB-EDR	36	192 GB	800 GB	20
SkyLake Superdome	Gold 6132	Flex Grid	14	6 TB	6 TB	8
AMD	EPYC 7501	IB-EDR	64	256 GB	800GB	4

Skylake compute node



System comparison

	Tier 2			
	ThinKing Cluster		Genius (2018)	
Total nodes	176 / 32	48 / 96	86 / 10	4
Processor type	Ivybridge	Haswell	Sky Lake	AMD
Base Clock Speed	2.8 GHz	2.5 GHz	2.3 GHz	2.0 GHz
Cores per node	20	24	36	64
Total cores	4,160	3,456	3,456	256
Memory per node (GB)	64 / 128	64 / 128	192 / 768	256
Memory per core (GB)	3.2 / 6.4	2.7 / 5.3	5.3 / 21.3	1
Memory bandwidth/socket	60 GB/s	68 GB/s	128GB/s	318GB/s
Peak performance (Flops/cycle)	4 DP FLOPs/cycle: 4-wide AVX addition OR multiplication	8 DP FLOPs/cycle: 4-wide FMA (fused multiply-add) instructions AVX2	16 DP FLOPs/cycle: 8-wide FMA (fused multiply-add) instructions AVX-512	instructions AVX-512
Network	Infiniband QDR 2:1	Infiniband FDR	Infiniband EDR	Infiniband EDR
Cache (L1 KB/L2 KB/L3 MB)	10x(32i+32d) / 10x256 / 25 MB	12x(32i+32d) / 12x256 / 30MB	18x(32i+32d) / 18x1024 / 25 MB	32x(64i+32d) / 32x512 / 64 MB

Storage

NetApp, DataDirect (DDN)

Overview of the storage infrastructure

HPC cluster storage at KU Leuven consists of 3 different storage types, optimized for different usage, with different characteristics

- NAS storage, fully back-up with snapshots for `home` and `data`
- `Scratch` storage, fast parallel filesystem
- `Archive` storage, to store large amounts of data for long time

Overview of the storage infrastructure

- Home directory (3GB)
  - Location available as `$VSC_HOME`
  - The data stored here should be relatively small (e.g., no files or directories larger than a gigabyte, although this is allowed), and not generating very intense I/O during jobs.
  - Typically all kinds of configuration files are stored here, e.g., ssh-keys, .bashrc, or Matlab, and Eclipse configuration, ...

Overview of the storage infrastructure

- Data directory (75 GB)
    - Location available as `$VSC_DATA`
    - A bigger 'workspace', for software, datasets, results, logfiles, ...
    - This filesystem can be used for higher I/O loads, but for I/O bound jobs, you might be better off using one of the 'scratch' filesystems.

Overview of the storage infrastructure

- Scratch directories (default: 100GB)
  - Free temporary upgrade of quota
  - For temporary or transient data; there is typically no backup for these filesystems, and 'old' data is removed automatically after 28 days (21 days is the duriation of longest job allowed on the cluster)
  - Currently `$VSC_SCRATCH` (`$VSC_SCRATCH_SITE`) are defined, for space that is available per user per site

Overview of the storage infrastructure

- Scratch directories (200GB)
  - `$VSC_SCRATCH_NODE` defined for space that is available per node (to be used only during the job execution, need to copy the data as everything will be erased after the job ends).

Tip:

- Do not use `/tmp` directory on compute node (very limited space ~10GB, once exceeded the system and your job will crash).
- Use `$VSC_SCRATCH_NODE` (`/local_scratch`) instead (~200GB)

Storage areas

Name	Variable	Type	Access	Backup	Quota
/user/leuven/30X/vsc30XXX	$VSC_HOME	NFS	Global	YES	3 GB
/data/leuven/30X/vsc30XXX	$VSC_DATA	NFS	Global	YES	75 GB
/scratch/leuven/30X/vsc30XXX	$VSC_SCRATCH $VSC_SCRATCH_SITE	GPFS	Global	NO	100 GB
/node_scratch (Genius)	$VSC_SCRATCH_NODE	ext4	Local	NO	200GB

Do not use /vsc-hard-mounts/leuven-data/… path instead (mount point can be changed)

Use /user/leuven/304/vsc30468 for $VSC_HOME
/data/leuven/304/vsc30468 for $VSC_DATA
/scratch/leuven/304/vsc30468 for $VSC_SCRATCH

To check available space:

- `$ myquota`
- `$ quota -s` ($VSC_HOME and $VSC_DATA)
- `$ mmlsquota --block-size auto vol_ddn2:leuven_scratch` ($VSC_SCRATCH)

Storage

- **Where to request**: https://admin.kuleuven.be/icts/onderzoek/hpc/hpc-storage.
- **More info**:

  https://icts.kuleuven.be/sc/english/research/HPC.

Login nodes

Access & data transfer, NX

Login Hosts on Different Machines/partitions

To login (with PuTTY or SSH client), you need VSC number and a hostname

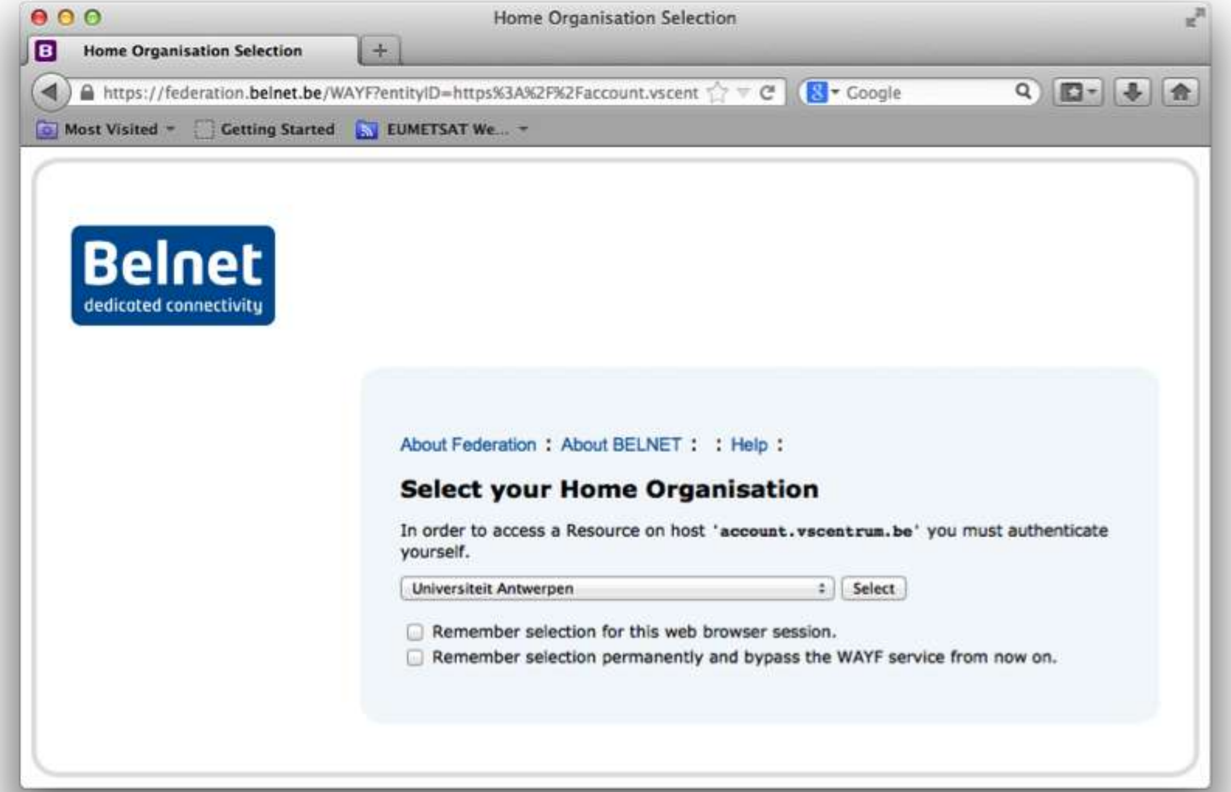
```
$ ssh -X vscXXXXX@<hostname>
```

Cluster / Partition	<hostname>	Remark(s)
ThinKing: IvyBridge	`login5-tier2.hpc.kuleuven.be` `login6-tier2.hpc.kuleuven.be`	
ThinKing: Haswell	`login7-tier2.hpc.kuleuven.be` `login8-tier2.hpc.kuleuven.be`	Visualization - TurboVNC
Genius	`login1-tier2.hpc.kuleuven.be` `login2-tier2.hpc.kuleuven.be`	
	`login3-tier2.hpc.kuleuven.be` `login4-tier2.hpc.kuleuven.be`	Visualization - NX
Genius: Superdome	Any Genius login node	`module load superdome`

- General login name:
- login.hpc.kuleuven.be → Genius
- login-genius.hpc.kuleuven.be
- login-thinking.hpc.kuleuven.be

Account request

- https://account.vscentrum.be/



Home Organisation Selection
Home Organisation Selection
https://federation.belnet.be/WAYF?entityID=https%3A%2F%2Faccount.vscent
Google
Most Visited
Getting Started
EUMETSAT We...
Belnet
dedicated connectivity

About Federation : About BELNET : : Help :

Select your Home Organisation

In order to access a Resource on host '`account.vscentrum.be`' you must authenticate yourself.

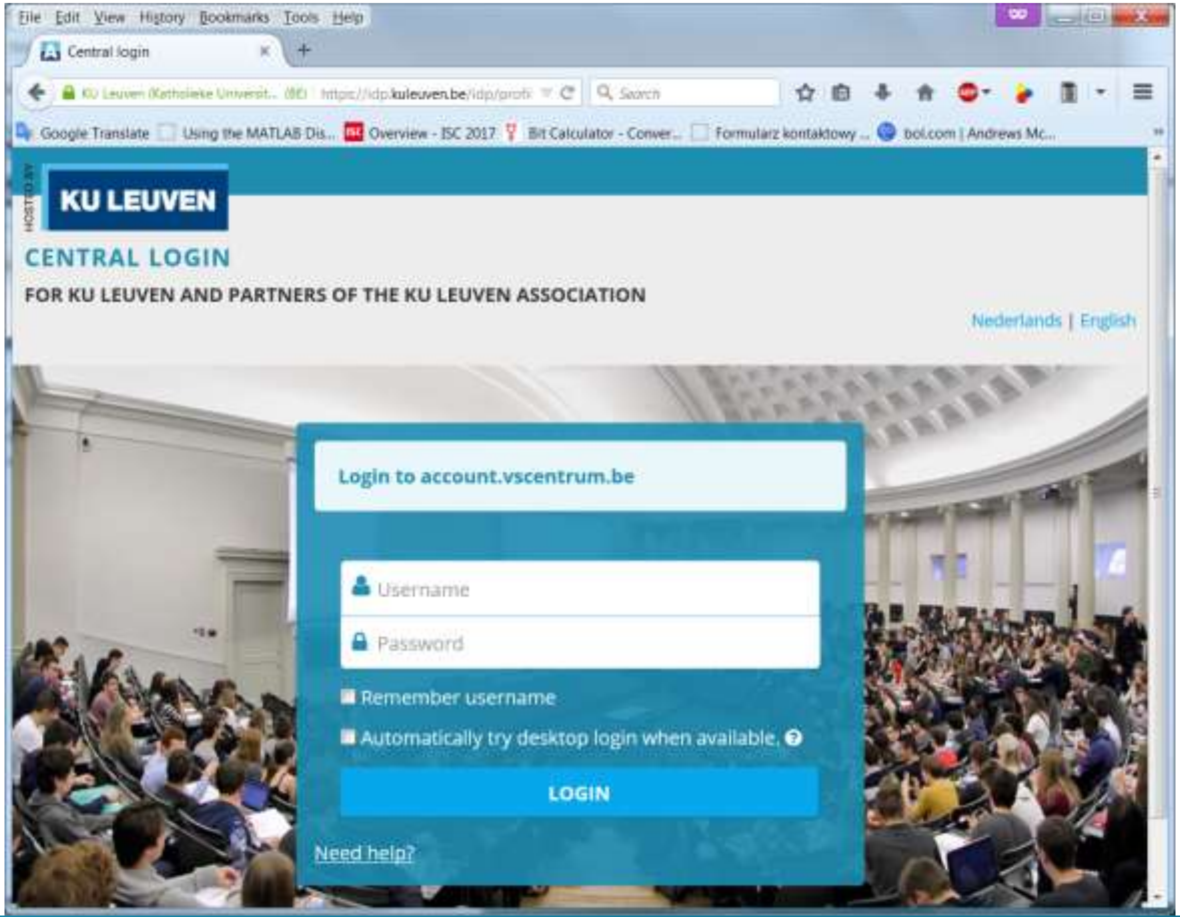
Universiteit Antwerpen [Select]

□ Remember selection for this web browser session.

□ Remember selection permanently and bypass the WAYF service from now on.

Account request

- https://account.vscentrum.be/
- KU Leuven


File Edit View History Bookmarks Tools Help
Central login
KU Leuven (Katholieke Universit... (BE) https://idp.kuleuven.be/idp/profi
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Bit Calculator - Conver...
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bol.com | Andrews Mc...
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KU LEUVEN

CENTRAL LOGIN

FOR KU LEUVEN AND PARTNERS OF THE KU LEUVEN ASSOCIATION

Nederlands | English

Login to account.vscentrum.be

Username

Password

□ Remember username

□ Automatically try desktop login when available.

LOGIN

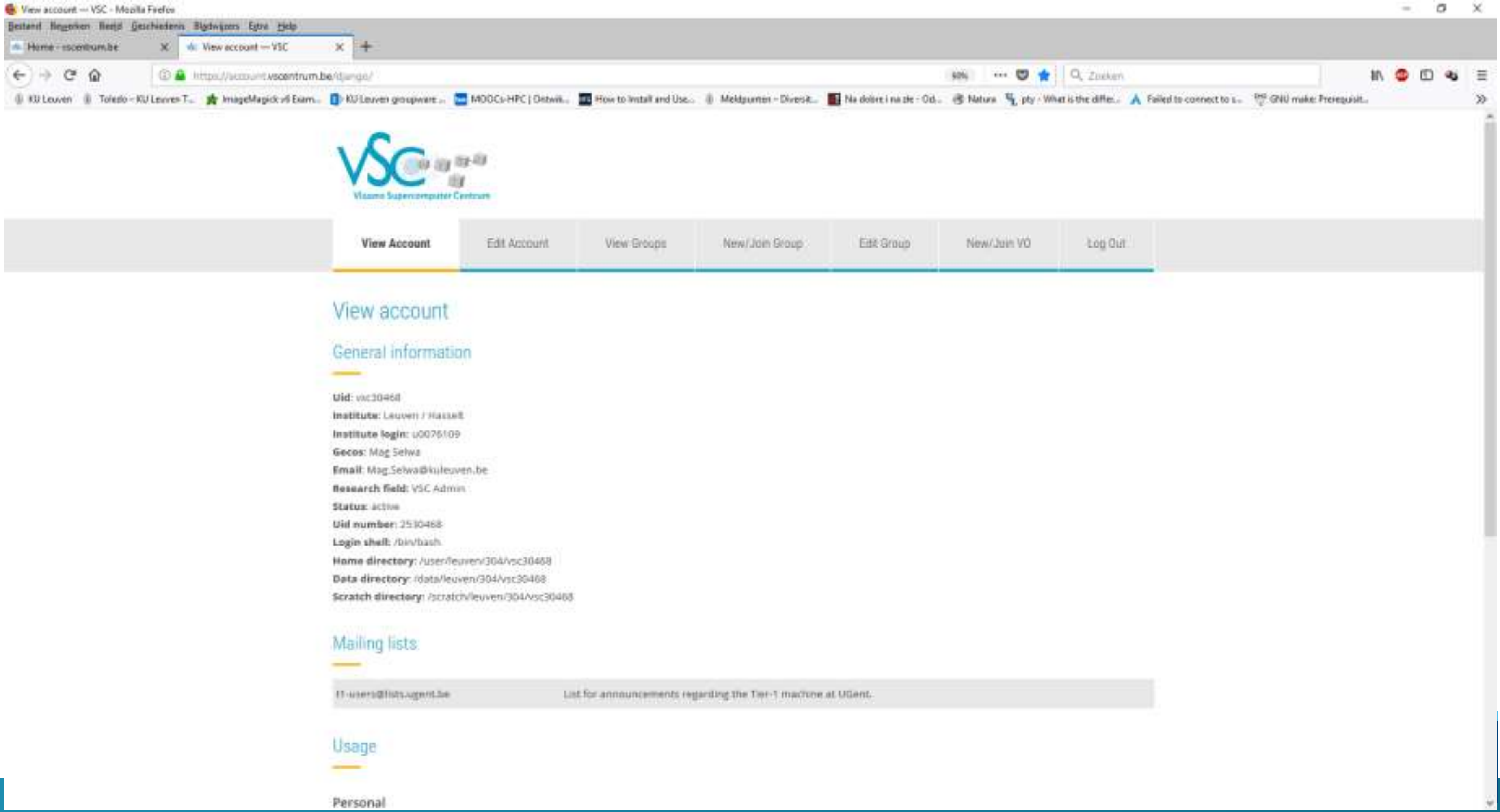
Need help?

Account request

- https://account.vscentrum.be/
- Authentication: Staff/student-id, e-mail
- In case of change – please inform us (access to the webpage may not be possible, SSH to the cluster not affected by that)

Account vs. VSC website

- https://account.vscentrum.be/


View account — VSC - Mozilla Firefox
Bestand Bewerken Beeld Geschiedenis Bladwijzers Extra Help
Home - vscentrum.be
View account — VSC
https://account.vscentrum.be/django/
Zoeken
Vlaams Supercomputer Centrum
View Account
Edit Account
View Groups
New/Join Group
Edit Group
New/Join VO
Log Out

View account

General information

Uid: vsc30468

Institute: Leuven / Hasselt

Institute login: u0076109

Gecos: Mag Selwa

Email: Mag.Selwa@kuleuven.be

Research field: VSC Admin

Status: active

Uid number: 2530468

Login shell: /bin/bash

Home directory: /user/leuven/304/vsc30468

Data directory: /data/leuven/304/vsc30468

Scratch directory: /scratch/leuven/304/vsc30468

Mailing lists

t1-users@lists.ugent.be	List for announcements regarding the Tier-1 machine at UGent.

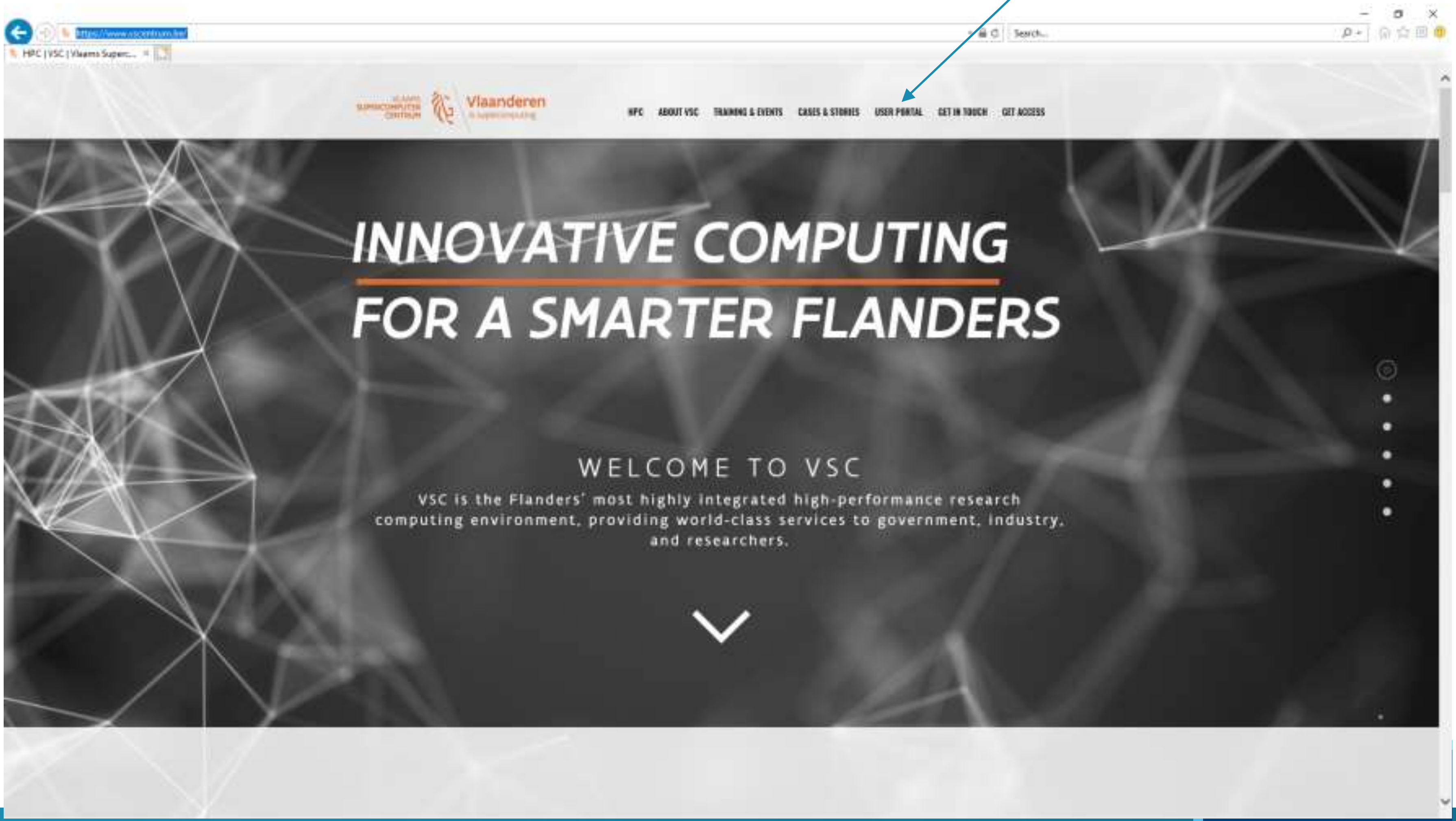
Usage

Personal

Account vs. VSC website

- https://www.vscentrum.be/

Help and info


https://www.vscentrum.be/
Search...
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VLAAMS SUPERCOMPUTER CENTRUM
Vlaanderen is supercomputing
HPC
ABOUT VSC
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CASES & STORIES
USER PORTAL
GET IN TOUCH
GET ACCESS

INNOVATIVE COMPUTING FOR A SMARTER FLANDERS

WELCOME TO VSC

VSC is the Flanders' most highly integrated high-performance research computing environment, providing world-class services to government, industry, and researchers.

I deleted my key…

- If the **private key** is deleted from your computer – you need to generate another pair and upload the public key through the account page
- If the **public key** is deleted from the cluster
  - go to the account webpage (https://account.vscentrum.be) and under ”Edit Account” reset SSH permissions
  - or upload it again through the account page
  - or contact us how to get the deleted files back to your directory
- I **forgot the passphrase** = I do not have a useful key pair = you need to generate another pair and upload the public key through the account page

I change the operating system…

- Update the system – nothing needs to be done
- Switch between Windows and Linux/Mac OS:
  - You may generate another key-pair and upload the public key through the account page
  - You can convert the existing private key so that your public key does not have to be replaced: https://vlaams-supercomputing-centrum-vscdocumentation.readthedocs-hosted.com/en/latest/_downloads/e7a2b5135d512681fdee66773cd88177/nx_config_guide.pdf

SSH overview

Private keys are always secret

- Anyone who can access your private key can log in as you!
- Set a passphrase on your private key
- Private key is encrypted with this passphrase
- Always a pair of keys is needed
- Both keys need to be generated together

Generate the key

Linux/Mac OS users:

- Use “*ssh-keygen ” command to generate key pair*
- **Be sure to give your key a passphrase!**
- Requested ssh key format: RSA 4096 bit

```
user@desktop:~> ssh-keygen -t rsa -b 4096
Generating public/private rsa key pair.
Enter file in which to save the key (/home/user/.ssh/id_rsa):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in /home/user/.ssh/id_rsa.
Your public key has been saved in /home/user/.ssh/id_rsa.pub.
The key fingerprint is:
f6:61:a8:27:35:cf:4c:6d:13:22:70:cf:4c:c8:a0:23
```

Generate the key

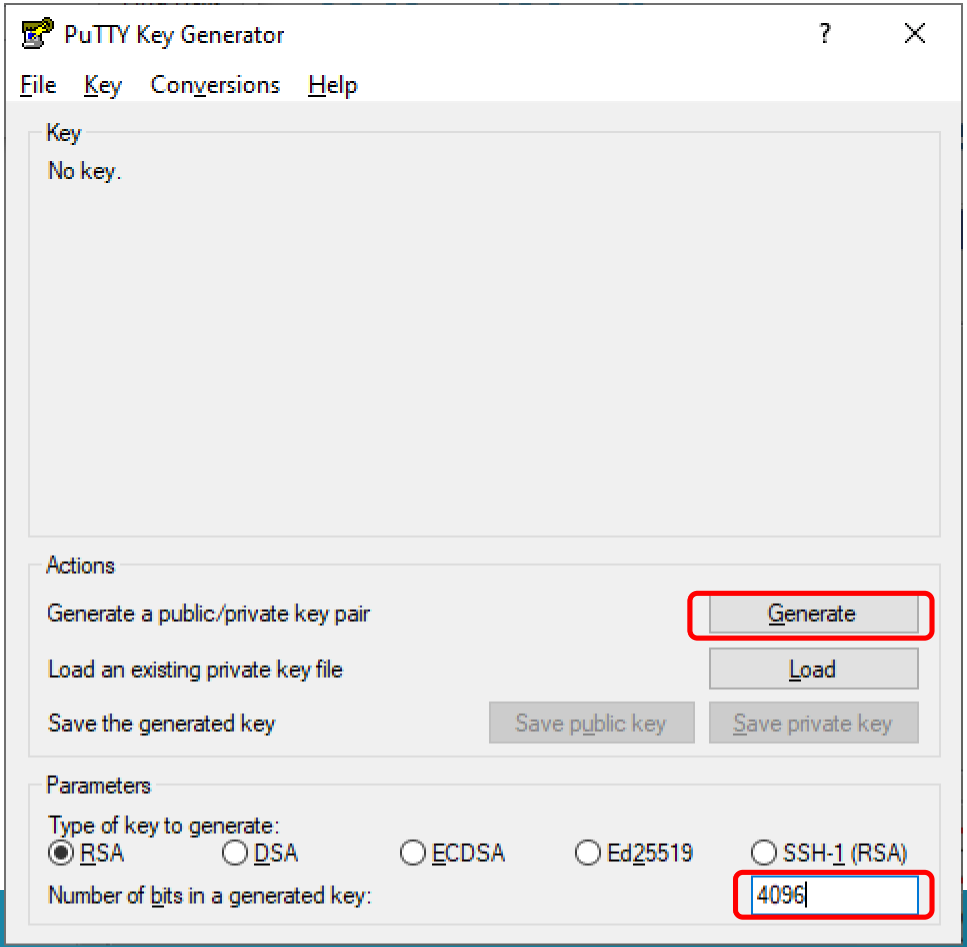
Linux/Mac OS users:

- Use “*ssh-keygen ” command to generate key pair*
- **Be sure to give your key a passphrase!**
- Default location: ~/.ssh/id_rsa (~/.ssh/id_rsa.pub)
- If other location: `ssh -i` *`localtion-of-the-file`* ……
- **keychain**: ssh agent to load the key with passphrase for current linux session

Generate the key

Windows users: use the PuTTYgen key generator.

Request ssh key format: RSA 4096 bit



PuTTY Key Generator

Key

No key.

Actions

Generate a public/private key pair

Load an existing private key file

Save the generated key

Parameters

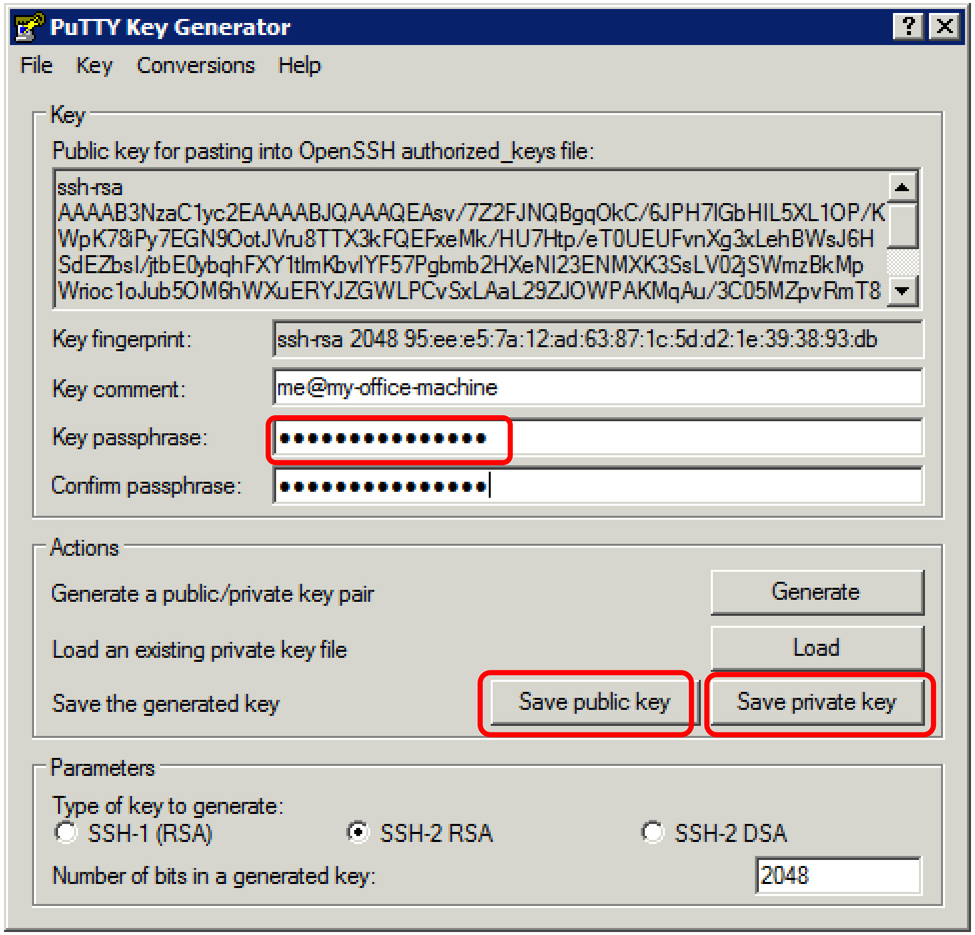
Type of key to generate:

● RSA ○ DSA ○ ECDSA ○ Ed25519 ○ SSH-1 (RSA)

Number of bits in a generated key: 4096

Generate the key

Be sure to give your key a passphrase!



Public key for pasting into OpenSSH authorized_keys file:

```
ssh-rsa
AAAAB3NzaC1yc2EAAAABJQAAAQEAsv/7Z2FJNQBgqOkC/6JPH7lGbHIL5XL1OP/K
WpK78iPy7EGN9OotJVru8TTX3kFQEFxeMk/HU7Htp/eT0UEUFvnXg3xLehBWsJ6H
SdEZbsl/jtbE0ybqhFXY1tlmKbvlYF57Pgbmb2HXeNI23ENMXK3SsLV02jSWmzBkMp
Wrioc1oJub5OM6hWXuERYJZGWLPCvSxLAaL29ZJOWPAKMqAu/3C05MZpvRmT8
```

Key fingerprint: ssh-rsa 2048 95:ee:e5:7a:12:ad:63:87:1c:5d:d2:1e:39:38:93:db

Key comment: me@my-office-machine

Key passphrase: ●●●●●●●●●●●●●●●

Confirm passphrase: ●●●●●●●●●●●●●●●

Generate a public/private key pair — Generate

Load an existing private key file — Load

Save the generated key — Save public key — Save private key

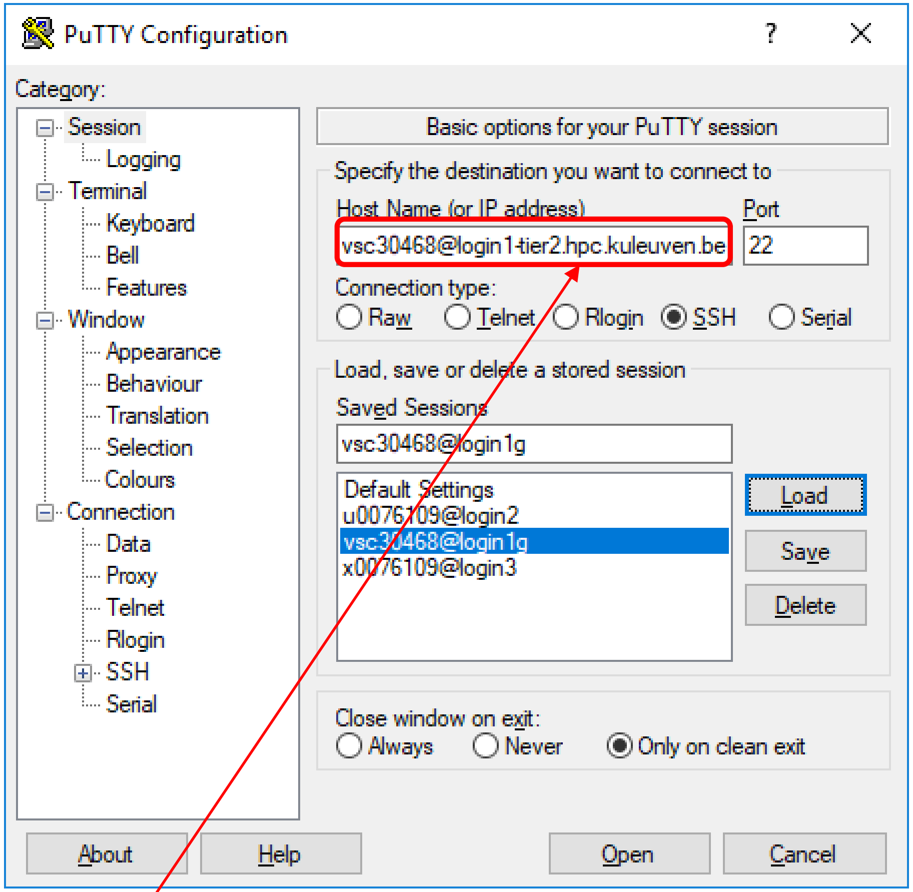
Type of key to generate:
○ SSH-1 (RSA) ● SSH-2 RSA ○ SSH-2 DSA

Number of bits in a generated key: 2048

Connecting to the cluster: text mode

Windows users:

- PuTTY is a simple-to-use and freely available GUI SSH client for Windows.
- Pageant can be used to manage active keys for PuTTY, WinSCP and FileZilla so that you don't need to enter the passphrase all the time.



PuTTY Configuration

Category:

Basic options for your PuTTY session

Specify the destination you want to connect to

Host Name (or IP address): vsc30468@login1-tier2.hpc.kuleuven.be

Port: 22

Connection type: ○ Raw ○ Telnet ○ Rlogin ● SSH ○ Serial

Load, save or delete a stored session

Saved Sessions: vsc30468@login1g

Default Settings
u0076109@login2
vsc30468@login1g
x0076109@login3

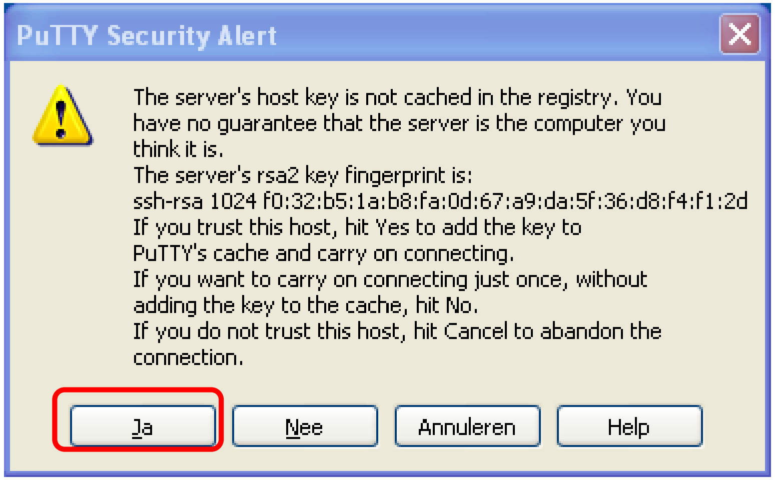
Close window on exit: ○ Always ○ Never ● Only on clean exit

vsc3XXXX@login1-tier2.hpc.kuleuven.be

Connecting to the cluster: text mode

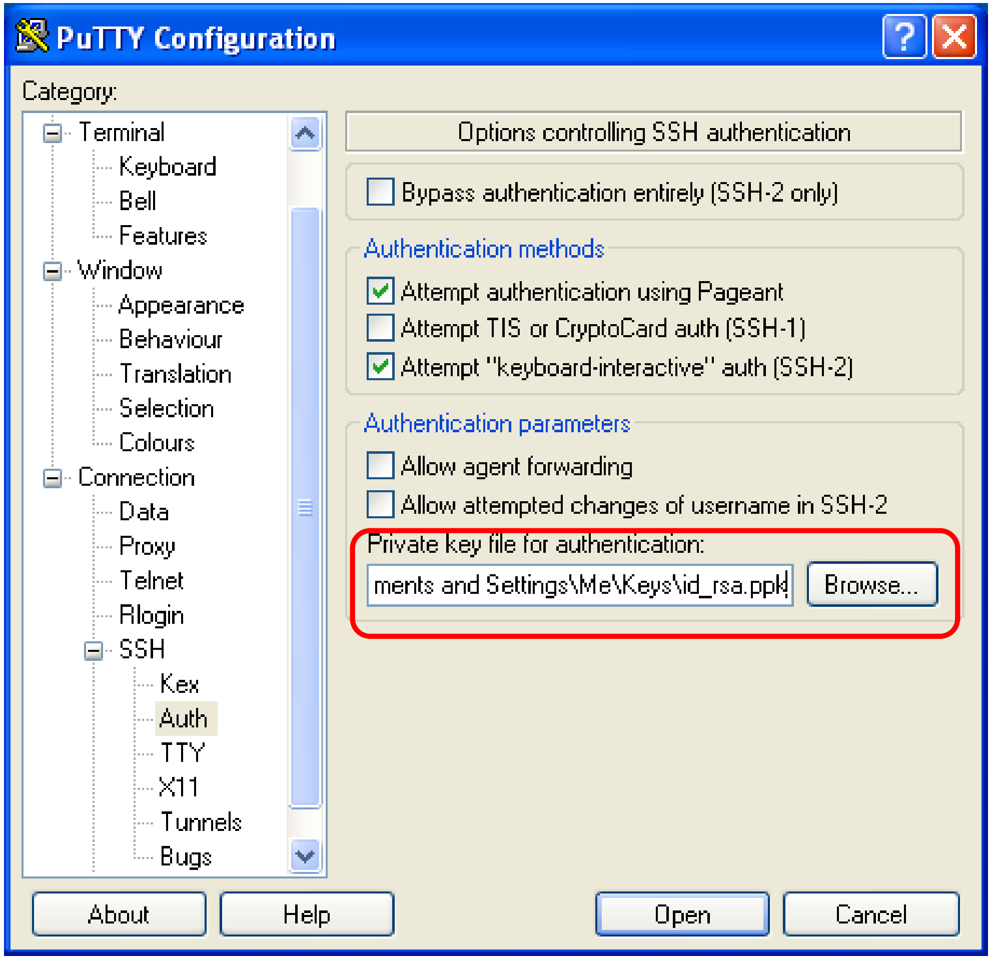
Windows users:

- PuTTY is a simple-to-use and freely available GUI SSH client for Windows.



PuTTY Security Alert

The server's host key is not cached in the registry. You have no guarantee that the server is the computer you think it is.
The server's rsa2 key fingerprint is:
ssh-rsa 1024 f0:32:b5:1a:b8:fa:0d:67:a9:da:5f:36:d8:f4:f1:2d
If you trust this host, hit Yes to add the key to PuTTY's cache and carry on connecting.
If you want to carry on connecting just once, without adding the key to the cache, hit No.
If you do not trust this host, hit Cancel to abandon the connection.



PuTTY Configuration

Options controlling SSH authentication

□ Bypass authentication entirely (SSH-2 only)

Authentication methods

☑ Attempt authentication using Pageant
□ Attempt TIS or CryptoCard auth (SSH-1)
☑ Attempt "keyboard-interactive" auth (SSH-2)

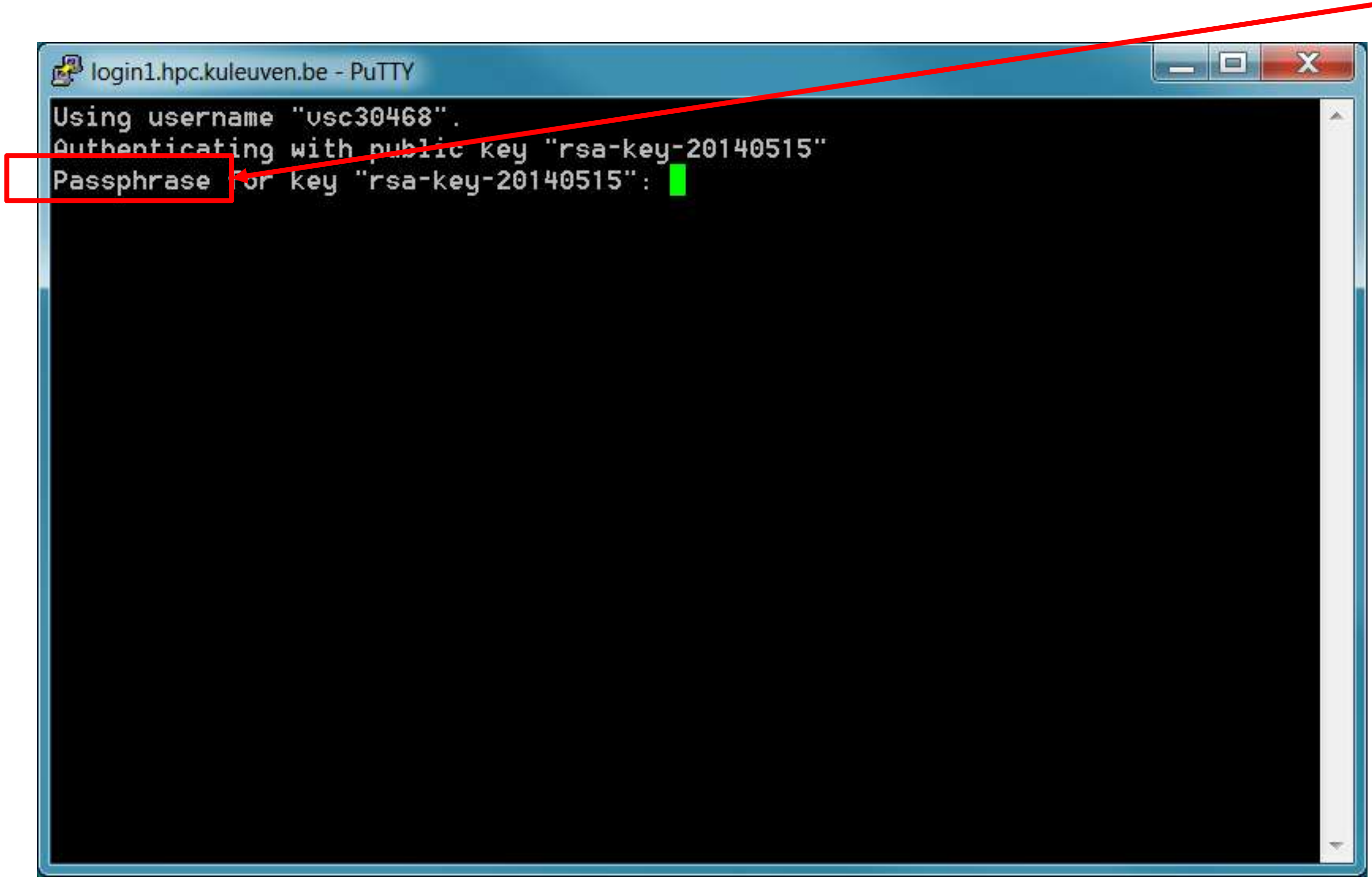
Authentication parameters

□ Allow agent forwarding
□ Allow attempted changes of username in SSH-2

Private key file for authentication:
ments and Settings\Me\Keys\id_rsa.ppk

Connecting to the cluster: text mode

Windows users:



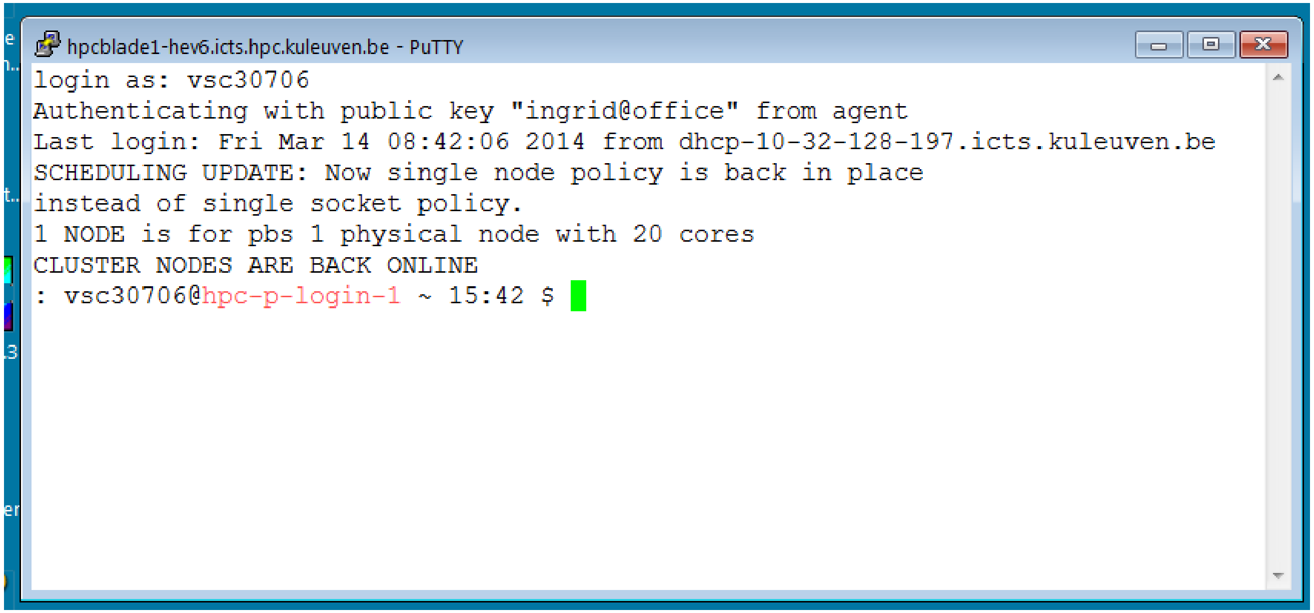
```
Using username "vsc30468".
Authenticating with public key "rsa-key-20140515"
Passphrase for key "rsa-key-20140515":
```

If asked for **password** no for passphrase – please stop connecting and contact suport, otherwise after a few attempts you will be blocked for 24hrs

How to get started?

- Linux users:

  ssh vsc3XXXX@login1-tier2.hpc.kuleuven.be



```
login as: vsc30706
Authenticating with public key "ingrid@office" from agent
Last login: Fri Mar 14 08:42:06 2014 from dhcp-10-32-128-197.icts.kuleuven.be
SCHEDULING UPDATE: Now single node policy is back in place
instead of single socket policy.
1 NODE is for pbs 1 physical node with 20 cores
CLUSTER NODES ARE BACK ONLINE
: vsc30706@hpc-p-login-1 ~ 15:42 $
```

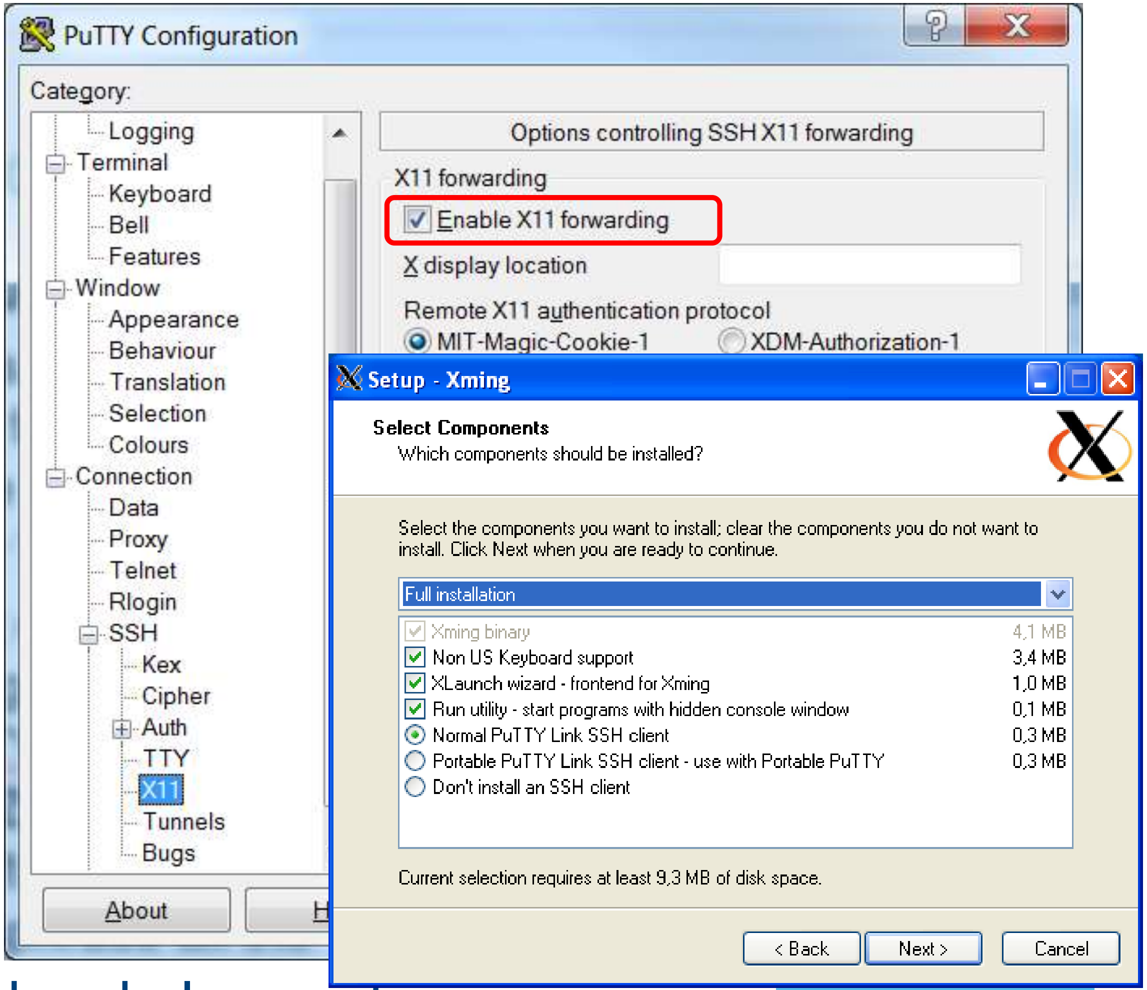
If asked for **password** no for passphrase – please stop connecting and contact suport, otherwise after a few attempts you will be blocked for 24hrs

… and you are in!

Connecting to the cluster: display graphics

Windows users:

- PuTTY is a simple-to-use and freely available GUI SSH client for Windows.
- Pageant can be used to manage active keys for PuTTY
- Xming: using X-windows to display graphical programs



PuTTY Configuration

Category:

Options controlling SSH X11 forwarding

X11 forwarding

☑ Enable X11 forwarding

X display location

Remote X11 authentication protocol

● MIT-Magic-Cookie-1 ○ XDM-Authorization-1

Setup - Xming

Select Components

Which components should be installed?

Select the components you want to install; clear the components you do not want to install. Click Next when you are ready to continue.

Full installation

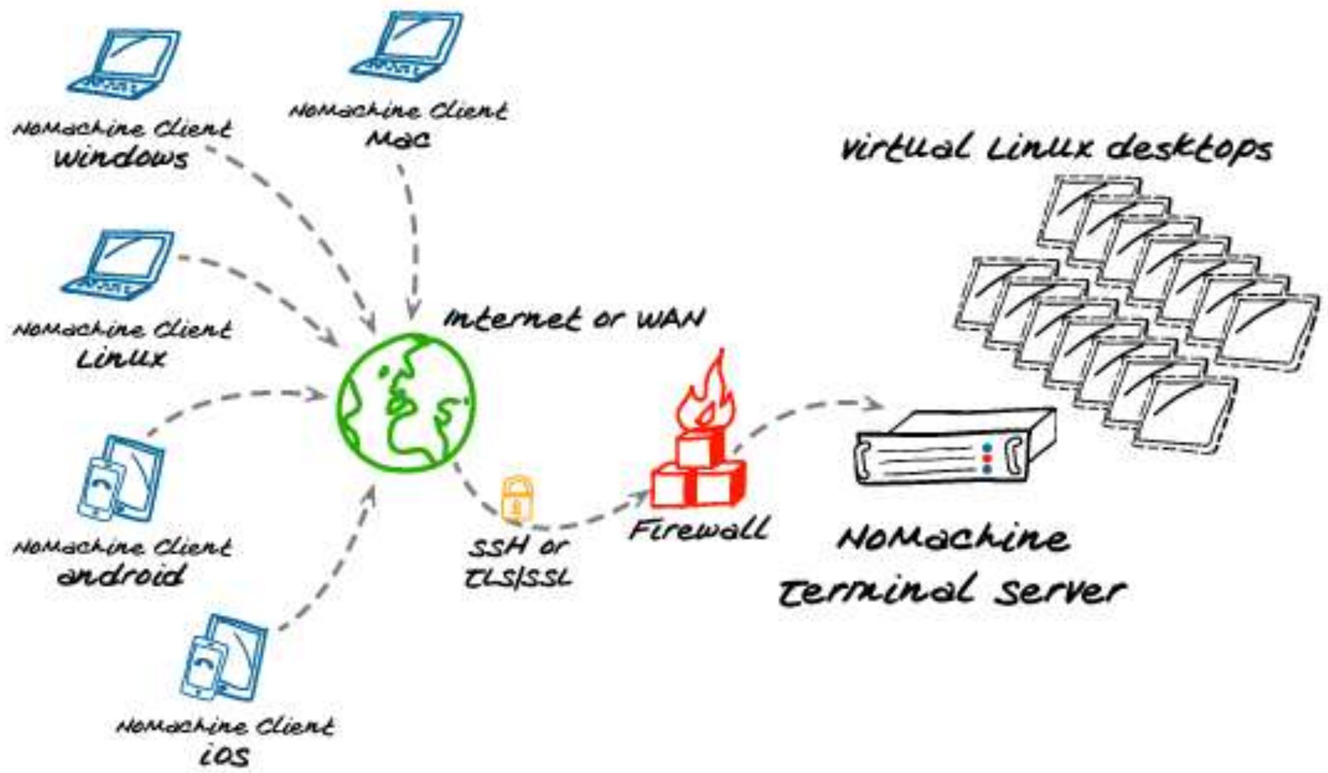
☑ Xming binary	4,1 MB
☑ Non US Keyboard support	3,4 MB
☑ XLaunch wizard - frontend for Xming	1,0 MB
☑ Run utility - start programs with hidden console window	0,1 MB
● Normal PuTTY Link SSH client	0,3 MB
○ Portable PuTTY Link SSH client - use with Portable PuTTY	0,3 MB
○ Don't install an SSH client	

Current selection requires at least 9,3 MB of disk space.

Linux users:

- ssh -X vsc3XXXX@login.hpc.kuleuven.be

What is NX?

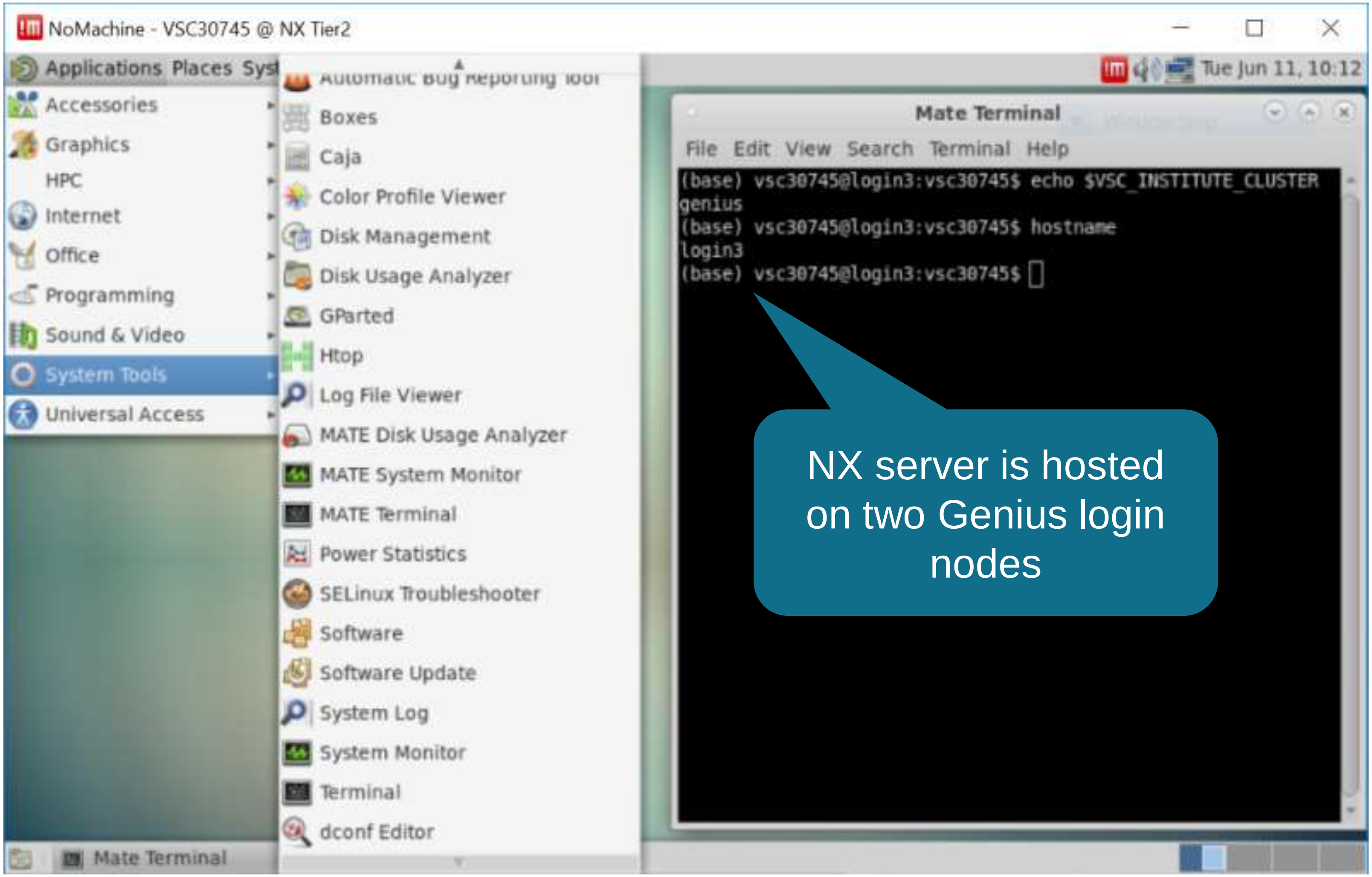


NX works by creating an nx-user on the server machine whose shell is executed any time a remote NX user connects to SSH using NX Client.

Main advantages of NX

- NX also allows to suspend and resume sessions and keeps session open (disconnected up to 30 days),
- During suspension, the processes invoked inside the session continue to run,
- Alternative for people using screen,
- More interactive jobs,
- Easy in use for editing, file management, developing software,
- Different limits of CPU (regular login node 36 min, NX node extended to 2 hrs).

NX virtual desktop



```
(base) vsc30745@login3:vsc30745$ echo $VSC_INSTITUTE_CLUSTER
genius
(base) vsc30745@login3:vsc30745$ hostname
login3
(base) vsc30745@login3:vsc30745$ 
```

NX server is hosted on two Genius login nodes

NX: available software

- **Accesories**: Gedit, Vi IMproved, Emacs (dummy version), Calculator,
- **Graphics**: gThumb (picture viewer), Xpdf Viewer,
- **Internet**: Firefox,
- **HPC**: **Computation**: Matlab (2018a), RStudio, SAS; **Visualisation**: Paraview, VisIt, VMD
- **Programming**: Meld Diff Viewer (visual diff and merge tool),
- **System tools**: File Browser, Terminal,
- **Additionally**: Gnuplot (graphing utility), Filezilla (file transfer tool), Evince (PDF, PostScript, TIFF, XPS, DVI Viewer),
- Software launched through modules from Terminal.

NX: How to get started

- https://vlaams-supercomputing-centrum-vscdocumentation.readthedocs-hosted.com/en/latest/access/nx_start_guide.html?highlight=nx
- **Configuration guide:** https://vlaams-supercomputing-centrum-vscdocumentation.readthedocs-hosted.com/en/latest/access/nx_start_guide.html?highlight=nx#nomachine-nx-client-configuration-guide

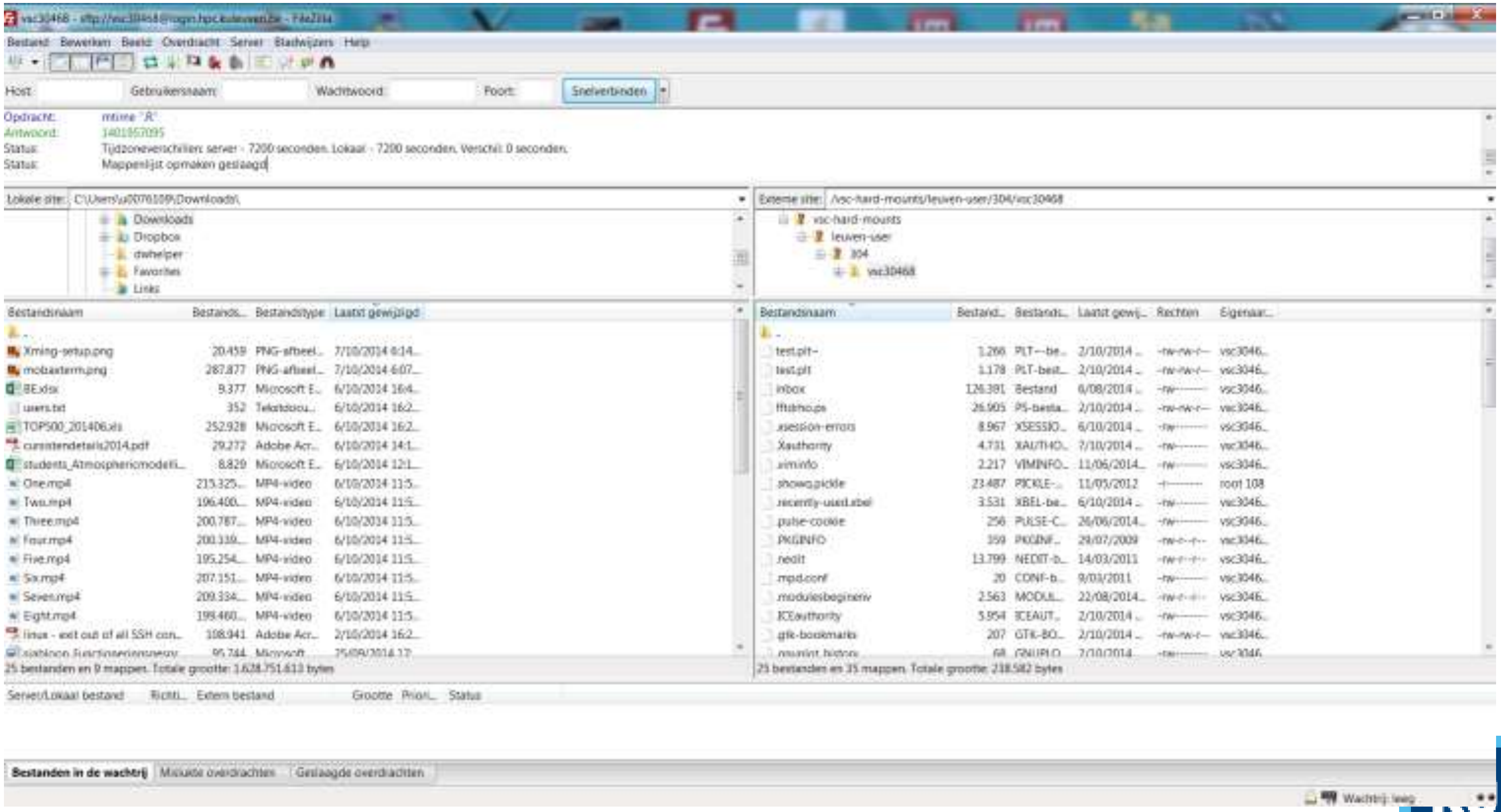
NX node is a login node (shared between other all the users).
Do not run your jobs there!

- **needs conversion of key for windows systems or pageant**

Connecting to the cluster: file transfer

Windows users:

- Filezilla (SFTP)
- WinSCP



```
Opdracht:    mtime ".R"
Antwoord:    1401957095
Status:      Tijdzoneverschillen: server: 7200 seconden. Lokaal: 7200 seconden. Verschil: 0 seconden.
Status:      Mappenlijst opmaken geslaagd
```

Lokale site: C:\Users\u0076109\Downloads\

- Downloads
- Dropbox
- dwhelper
- Favorites
- Links

Bestandsnaam	Bestands...	Bestandstype	Laatst gewijzigd
..			
Xming-setup.png	20.459	PNG-afbeel...	7/10/2014 6:14...
mobaxterm.png	287.877	PNG-afbeel...	7/10/2014 6:07...
BE.xlsx	9.377	Microsoft E...	6/10/2014 16:4...
users.txt	352	Tekstdocu...	6/10/2014 16:2...
TOP500_201406.xls	252.928	Microsoft E...	6/10/2014 16:2...
cursistendetails2014.pdf	29.272	Adobe Acr...	6/10/2014 14:1...
students_Atmosphericmodelli...	8.829	Microsoft E...	6/10/2014 12:1...
One.mp4	215.325...	MP4-video	6/10/2014 11:5...
Two.mp4	196.400...	MP4-video	6/10/2014 11:5...
Three.mp4	200.787...	MP4-video	6/10/2014 11:5...
Four.mp4	200.339...	MP4-video	6/10/2014 11:5...
Five.mp4	195.254...	MP4-video	6/10/2014 11:5...
Six.mp4	207.151...	MP4-video	6/10/2014 11:5...
Seven.mp4	209.334...	MP4-video	6/10/2014 11:5...
Eight.mp4	199.460...	MP4-video	6/10/2014 11:5...
linux - exit out of all SSH con...	108.941	Adobe Acr...	2/10/2014 16:2...
sjabloon Functioneringsgesp...	95.744	Microsoft ...	25/09/2014 12:...

25 bestanden en 9 mappen. Totale grootte: 1.628.751.613 bytes

Externe site: /vsc-hard-mounts/leuven-user/304/vsc30468

- vsc-hard-mounts
  - leuven-user
    - 304
      - vsc30468

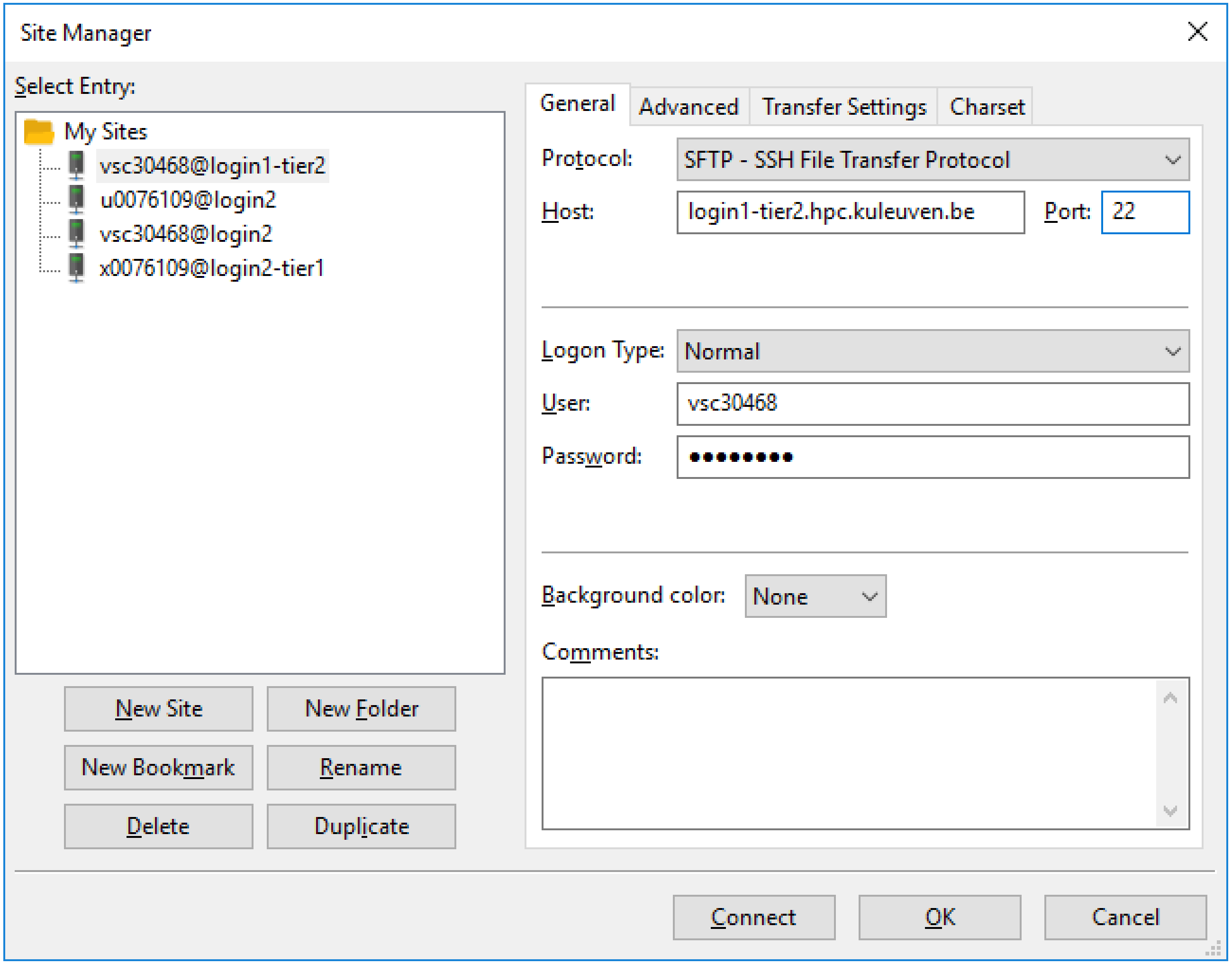
Bestandsnaam	Bestand...	Bestands...	Laatst gewij...	Rechten	Eigenaar...
..					
test.plt~	1.268	PLT~-be...	2/10/2014 ...	-rw-rw-r--	vsc3046...
test.plt	1.178	PLT-best...	2/10/2014 ...	-rw-rw-r--	vsc3046...
inbox	126.391	Bestand	6/08/2014 ...	-rw-------	vsc3046...
fftdrho.ps	26.905	PS-besta...	2/10/2014 ...	-rw-rw-r--	vsc3046...
.xsession-errors	8.967	XSESSIO...	6/10/2014 ...	-rw-------	vsc3046...
.Xauthority	4.731	XAUTHO...	7/10/2014 ...	-rw-------	vsc3046...
.viminfo	2.217	VIMINFO...	11/06/2014...	-rw-------	vsc3046...
.showq.pickle	23.487	PICKLE-...	11/05/2012	-r--------	root 108
.recently-used.xbel	3.531	XBEL-be...	6/10/2014 ...	-rw-------	vsc3046...
.pulse-cookie	256	PULSE-C...	26/06/2014...	-rw-------	vsc3046...
PKGINFO	359	PKGINF...	29/07/2009	-rw-r--r--	vsc3046...
.nedit	13.799	NEDIT-b...	14/03/2011	-rw-r--r--	vsc3046...
.mpd.conf	20	CONF-b...	9/03/2011	-rw-------	vsc3046...
.modulesbeginenv	2.563	MODUL...	22/08/2014...	-rw-r--r--	vsc3046...
.ICEauthority	5.954	ICEAUT...	2/10/2014 ...	-rw-------	vsc3046...
.gtk-bookmarks	207	GTK-BO...	2/10/2014 ...	-rw-rw-r--	vsc3046...
.gnuplot_history	68	GNUPLO...	2/10/2014 ...	-rw-------	vsc3046...

25 bestanden en 35 mappen. Totale grootte: 218.582 bytes

Connecting to the cluster: file transfer

Windows users:

- Filezilla (SFTP)



Site Manager

Select Entry:

- My Sites
  - vsc30468@login1-tier2
  - u0076109@login2
  - vsc30468@login2
  - x0076109@login2-tier1

Protocol: SFTP - SSH File Transfer Protocol

Host: login1-tier2.hpc.kuleuven.be Port: 22

Logon Type: Normal

User: vsc30468

Password: ●●●●●●●●●

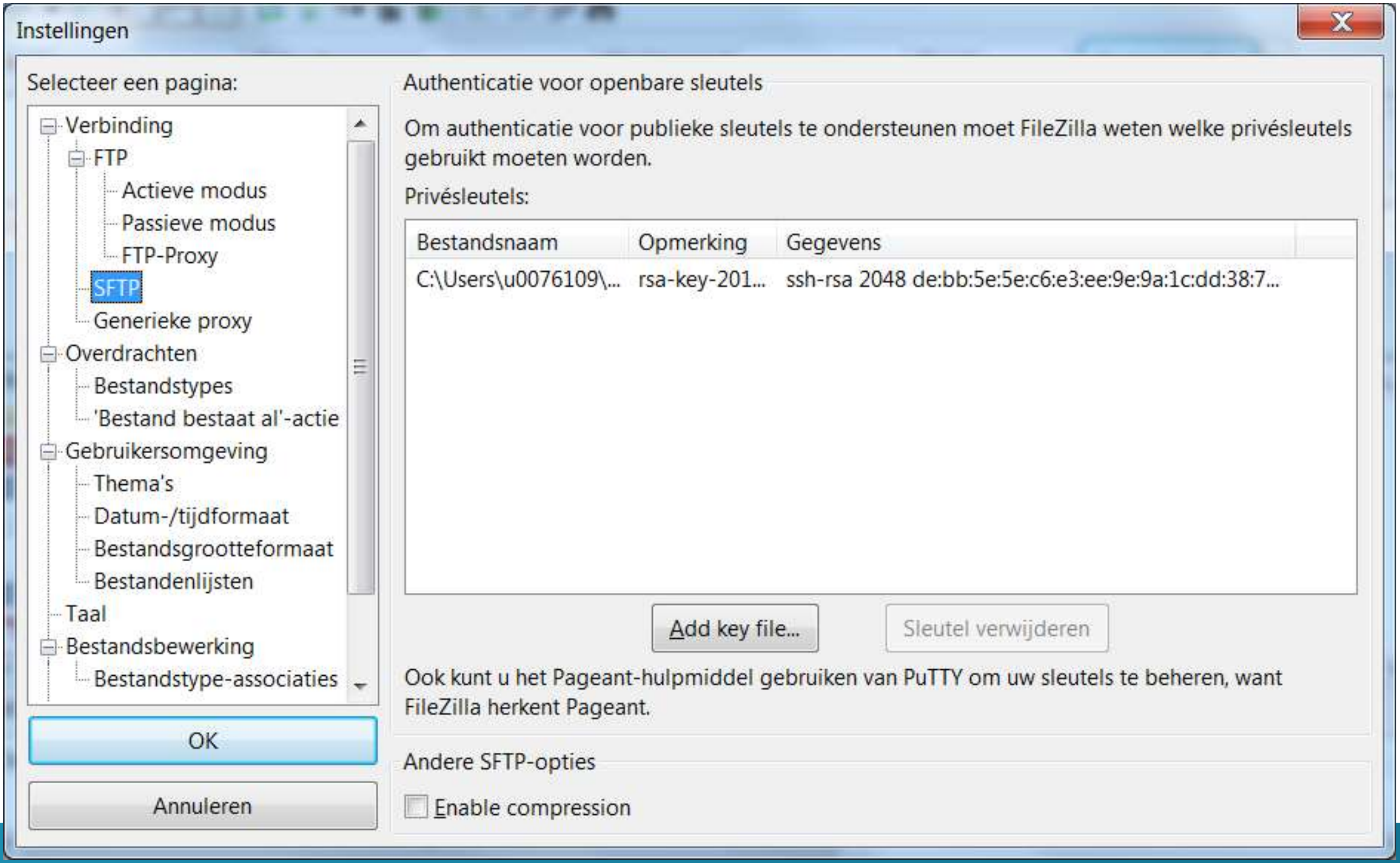
Background color: None

Comments:

Connecting to the cluster: file transfer

Windows users:

- Filezilla (SFTP)



Instellingen

Selecteer een pagina:

Authenticatie voor openbare sleutels

Om authenticatie voor publieke sleutels te ondersteunen moet FileZilla weten welke privésleutels gebruikt moeten worden.

Privésleutels:

Bestandsnaam	Opmerking	Gegevens
C:\Users\u0076109\...	rsa-key-201...	ssh-rsa 2048 de:bb:5e:5e:c6:e3:ee:9e:9a:1c:dd:38:7...

Ook kunt u het Pageant-hulpmiddel gebruiken van PuTTY om uw sleutels te beheren, want FileZilla herkent Pageant.

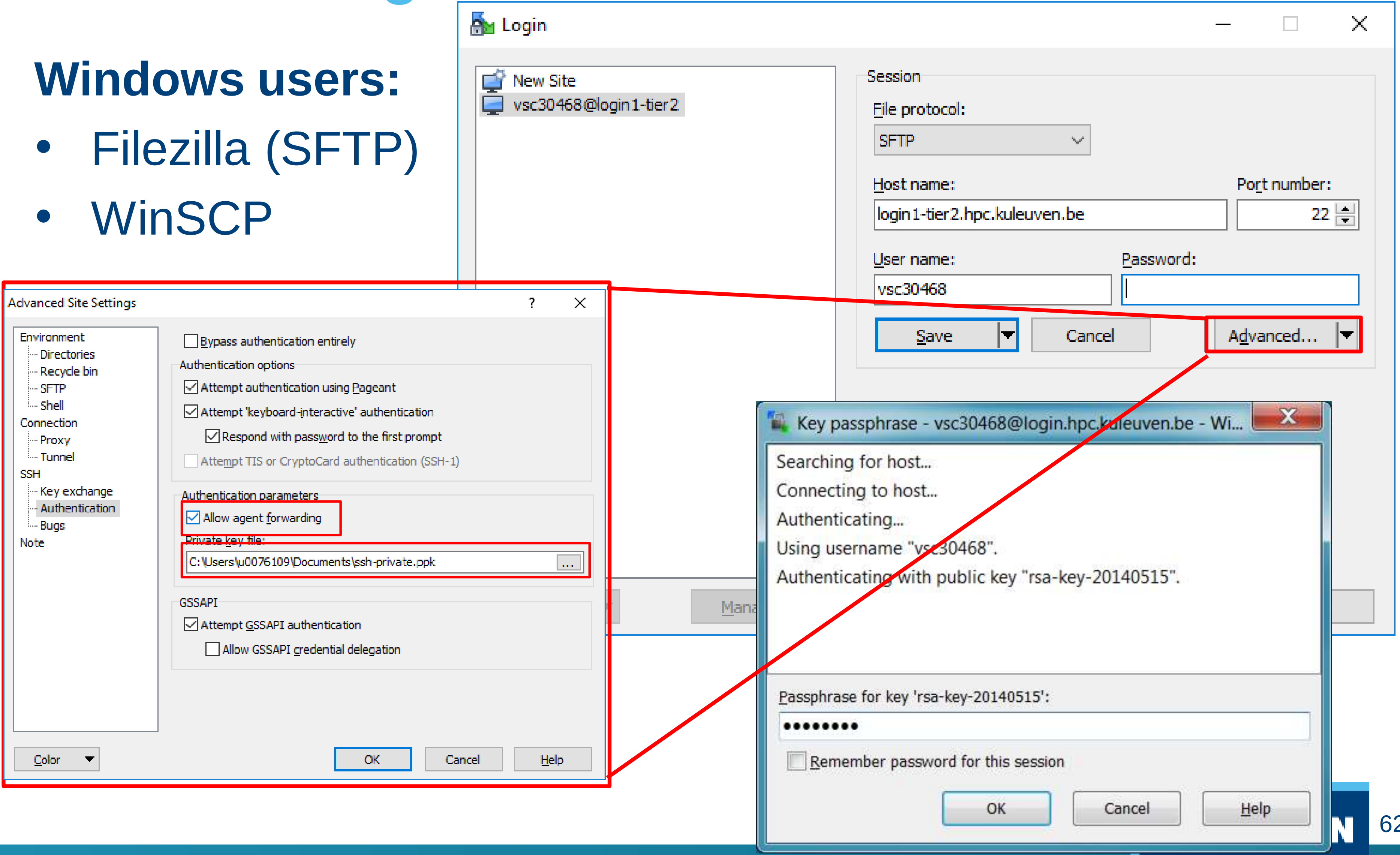
Andere SFTP-opties

□ Enable compression

Connecting to the cluster: file transfer

Windows users:

- Filezilla (SFTP)
- WinSCP



Login

- New Site
- vsc30468@login1-tier2

Session

File protocol: SFTP

Host name: login1-tier2.hpc.kuleuven.be

Port number: 22

User name: vsc30468

Password:

Advanced Site Settings

☐ Bypass authentication entirely

Authentication options

☑ Attempt authentication using Pageant

☑ Attempt 'keyboard-interactive' authentication

☑ Respond with password to the first prompt

☐ Attempt TIS or CryptoCard authentication (SSH-1)

Authentication parameters

☑ Allow agent forwarding

Private key file: C:\Users\u0076109\Documents\ssh-private.ppk

GSSAPI

☑ Attempt GSSAPI authentication

☐ Allow GSSAPI credential delegation

Key passphrase - vsc30468@login.hpc.kuleuven.be - Wi...

```
Searching for host...
Connecting to host...
Authenticating...
Using username "vsc30468".
Authenticating with public key "rsa-key-20140515".
```

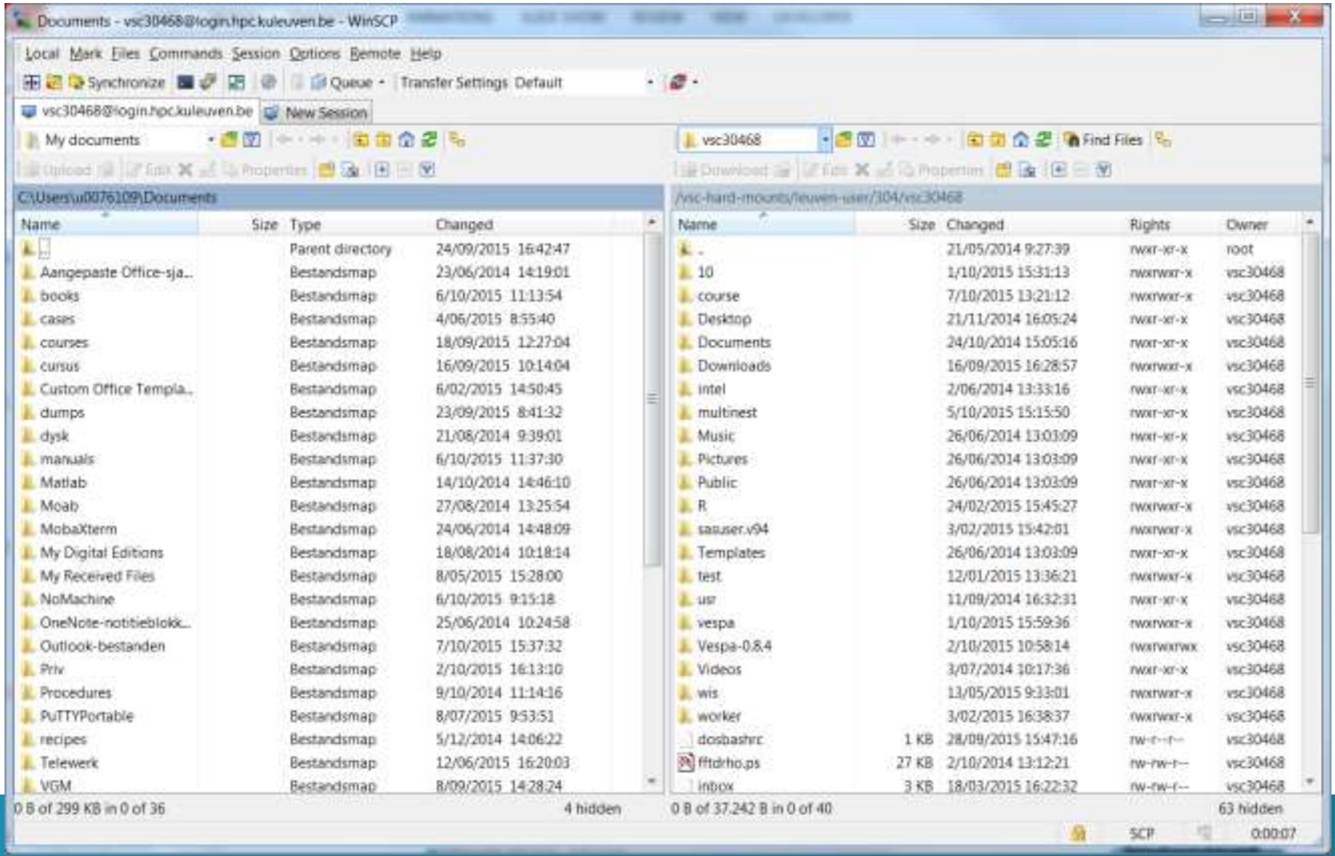
Passphrase for key 'rsa-key-20140515': ••••••••

☐ Remember password for this session

Connecting to the cluster: file transfer

Windows users:

- Filezilla (SFTP)
- WinSCP



Documents - vsc30468@login.hpc.kuleuven.be - WinSCP

Local Mark Files Commands Session Options Remote Help
Synchronize
Queue
Transfer Settings Default
vsc30468@login.hpc.kuleuven.be
New Session
My documents
Upload
Edit
Properties
vsc30468
Find Files
Download
Edit
Properties
SCP

C:\Users\u0076109\Documents

Name	Size	Type	Changed
..		Parent directory	24/09/2015 16:42:47
Aangepaste Office-sja...		Bestandsmap	23/06/2014 14:19:01
books		Bestandsmap	6/10/2015 11:13:54
cases		Bestandsmap	4/06/2015 8:55:40
courses		Bestandsmap	18/09/2015 12:27:04
cursus		Bestandsmap	16/09/2015 10:14:04
Custom Office Templa...		Bestandsmap	6/02/2015 14:50:45
dumps		Bestandsmap	23/09/2015 8:41:32
dysk		Bestandsmap	21/08/2014 9:39:01
manuals		Bestandsmap	6/10/2015 11:37:30
Matlab		Bestandsmap	14/10/2014 14:46:10
Moab		Bestandsmap	27/08/2014 13:25:54
MobaXterm		Bestandsmap	24/06/2014 14:48:09
My Digital Editions		Bestandsmap	18/08/2014 10:18:14
My Received Files		Bestandsmap	8/05/2015 15:28:00
NoMachine		Bestandsmap	6/10/2015 9:15:18
OneNote-notitieblokk...		Bestandsmap	25/06/2014 10:24:58
Outlook-bestanden		Bestandsmap	7/10/2015 15:37:32
Priv		Bestandsmap	2/10/2015 16:13:10
Procedures		Bestandsmap	9/10/2014 11:14:16
PuTTYPortable		Bestandsmap	8/07/2015 9:53:51
recipes		Bestandsmap	5/12/2014 14:06:22
Telewerk		Bestandsmap	12/06/2015 16:20:03
VGM		Bestandsmap	8/09/2015 14:28:24

0 B of 299 KB in 0 of 36 4 hidden

/vsc-hard-mounts/leuven-user/304/vsc30468

Name	Size	Changed	Rights	Owner
..		21/05/2014 9:27:39	rwxr-xr-x	root
10		1/10/2015 15:31:13	rwxrwxr-x	vsc30468
course		7/10/2015 13:21:12	rwxrwxr-x	vsc30468
Desktop		21/11/2014 16:05:24	rwxr-xr-x	vsc30468
Documents		24/10/2014 15:05:16	rwxr-xr-x	vsc30468
Downloads		16/09/2015 16:28:57	rwxrwxr-x	vsc30468
intel		2/06/2014 13:33:16	rwxr-xr-x	vsc30468
multinest		5/10/2015 15:15:50	rwxr-xr-x	vsc30468
Music		26/06/2014 13:03:09	rwxr-xr-x	vsc30468
Pictures		26/06/2014 13:03:09	rwxr-xr-x	vsc30468
Public		26/06/2014 13:03:09	rwxr-xr-x	vsc30468
R		24/02/2015 15:45:27	rwxrwxr-x	vsc30468
sasuser.v94		3/02/2015 15:42:01	rwxrwxr-x	vsc30468
Templates		26/06/2014 13:03:09	rwxr-xr-x	vsc30468
test		12/01/2015 13:36:21	rwxrwxr-x	vsc30468
usr		11/09/2014 16:32:31	rwxr-xr-x	vsc30468
vespa		1/10/2015 15:59:36	rwxrwxr-x	vsc30468
Vespa-0.8.4		2/10/2015 10:58:14	rwxrwxrwx	vsc30468
Videos		3/07/2014 10:17:36	rwxr-xr-x	vsc30468
wis		13/05/2015 9:33:01	rwxrwxr-x	vsc30468
worker		3/02/2015 16:38:37	rwxrwxr-x	vsc30468
dosbashrc	1 KB	28/09/2015 15:47:16	rw-r--r--	vsc30468
fftdrho.ps	27 KB	2/10/2014 13:12:21	rw-rw-r--	vsc30468
inbox	3 KB	18/03/2015 16:22:32	rw-rw-r--	vsc30468

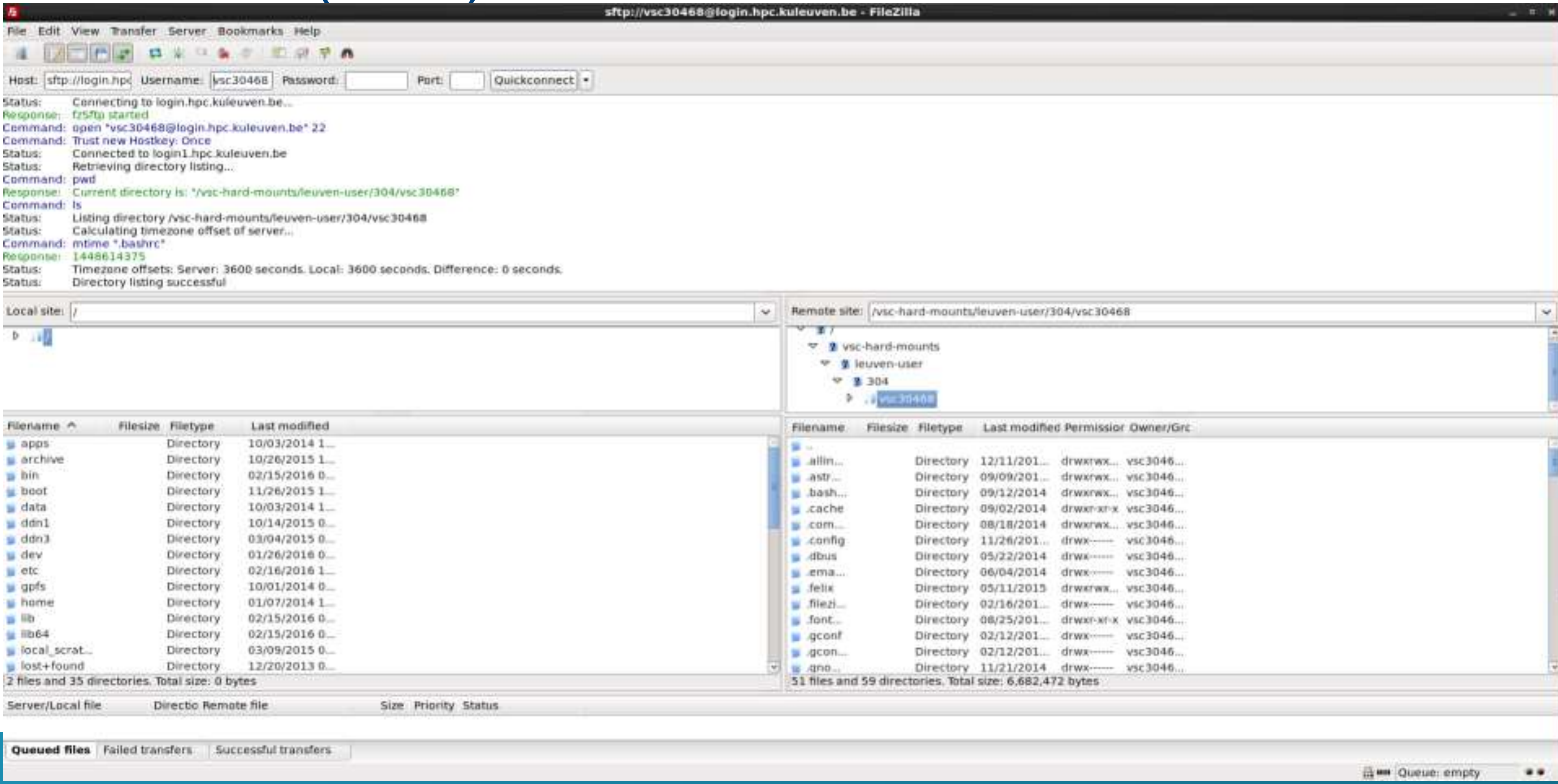
0 B of 37.242 B in 0 of 40 63 hidden

0:00:07

Connecting to the cluster: file transfer

Linux/Mac users:

- Filezilla (SFTP)



Host: sftp://login.hpc Username: vsc30468 Password: Port:

```
Status:     Connecting to login.hpc.kuleuven.be...
Response:   fzSftp started
Command:    open "vsc30468@login.hpc.kuleuven.be" 22
Command:    Trust new Hostkey: Once
Status:     Connected to login1.hpc.kuleuven.be
Status:     Retrieving directory listing...
Command:    pwd
Response:   Current directory is: "/vsc-hard-mounts/leuven-user/304/vsc30468"
Command:    ls
Status:     Listing directory /vsc-hard-mounts/leuven-user/304/vsc30468
Status:     Calculating timezone offset of server...
Command:    mtime ".bashrc"
Response:   1448614375
Status:     Timezone offsets: Server: 3600 seconds. Local: 3600 seconds. Difference: 0 seconds.
Status:     Directory listing successful
```

Local site: /

Remote site: /vsc-hard-mounts/leuven-user/304/vsc30468

```
/
  vsc-hard-mounts
    leuven-user
      304
        vsc30468
```

Filename	Filesize	Filetype	Last modified
apps		Directory	10/03/2014 1...
archive		Directory	10/26/2015 1...
bin		Directory	02/15/2016 0...
boot		Directory	11/26/2015 1...
data		Directory	10/03/2014 1...
ddn1		Directory	10/14/2015 0...
ddn3		Directory	03/04/2015 0...
dev		Directory	01/26/2016 0...
etc		Directory	02/16/2016 1...
gpfs		Directory	10/01/2014 0...
home		Directory	01/07/2014 1...
lib		Directory	02/15/2016 0...
lib64		Directory	02/15/2016 0...
local_scrat...		Directory	03/09/2015 0...
lost+found		Directory	12/20/2013 0...

2 files and 35 directories. Total size: 0 bytes

Filename	Filesize	Filetype	Last modified	Permissior	Owner/Grc
..					
.allin...		Directory	12/11/201...	drwxrwx...	vsc3046...
.astr...		Directory	09/09/201...	drwxrwx...	vsc3046...
.bash...		Directory	09/12/2014	drwxrwx...	vsc3046...
.cache		Directory	09/02/2014	drwxr-xr-x	vsc3046...
.com...		Directory	08/18/2014	drwxrwx...	vsc3046...
.config		Directory	11/26/201...	drwx------	vsc3046...
.dbus		Directory	05/22/2014	drwx------	vsc3046...
.ema...		Directory	06/04/2014	drwx------	vsc3046...
.felix		Directory	05/11/2015	drwxrwx...	vsc3046...
.filezi...		Directory	02/16/201...	drwx------	vsc3046...
.font...		Directory	08/25/201...	drwxr-xr-x	vsc3046...
.gconf		Directory	02/12/201...	drwx------	vsc3046...
.gcon...		Directory	02/12/201...	drwx------	vsc3046...
.gno...		Directory	11/21/2014	drwx------	vsc3046...

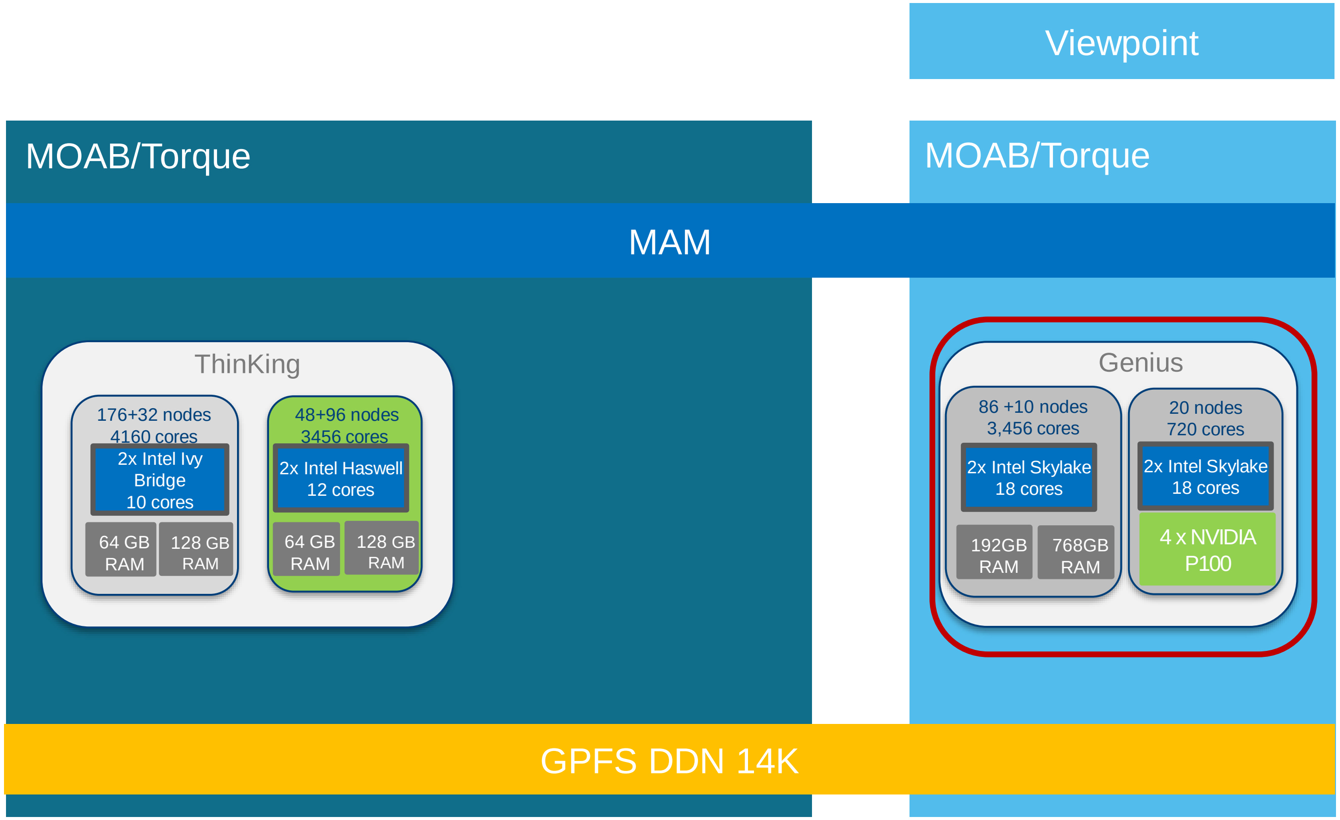
51 files and 59 directories. Total size: 6,682,472 bytes

Server/Local file	Directio	Remote file	Size	Priority	Status

Hands-on 1

- Login on the account webpage https://account.vscentrum.be/ and join the lp_hpcinfo_training group
- Login to the cluster
- Check your available space in $VSC_HOME, VSC_DATA and $VSC_SCRATCH directory

Production phase



Jobs need to be submitted separately to Thinking or Genius from login nodes

Torque/Moab - Genius

- **Jobs have to be submitted from new (Genius) login nodes**
- Some commands:
  - `$ qsub …` : Submit a job, returns a job ID

    ```
    $ qsub test.sh
    50001435.tier2-p-moab-2.icts.hpc.kuleuven.be
    ```

  - `$ qdel <job-id>` : Delete a queued or running job

    ```
    $ qdel 50001435
    ```

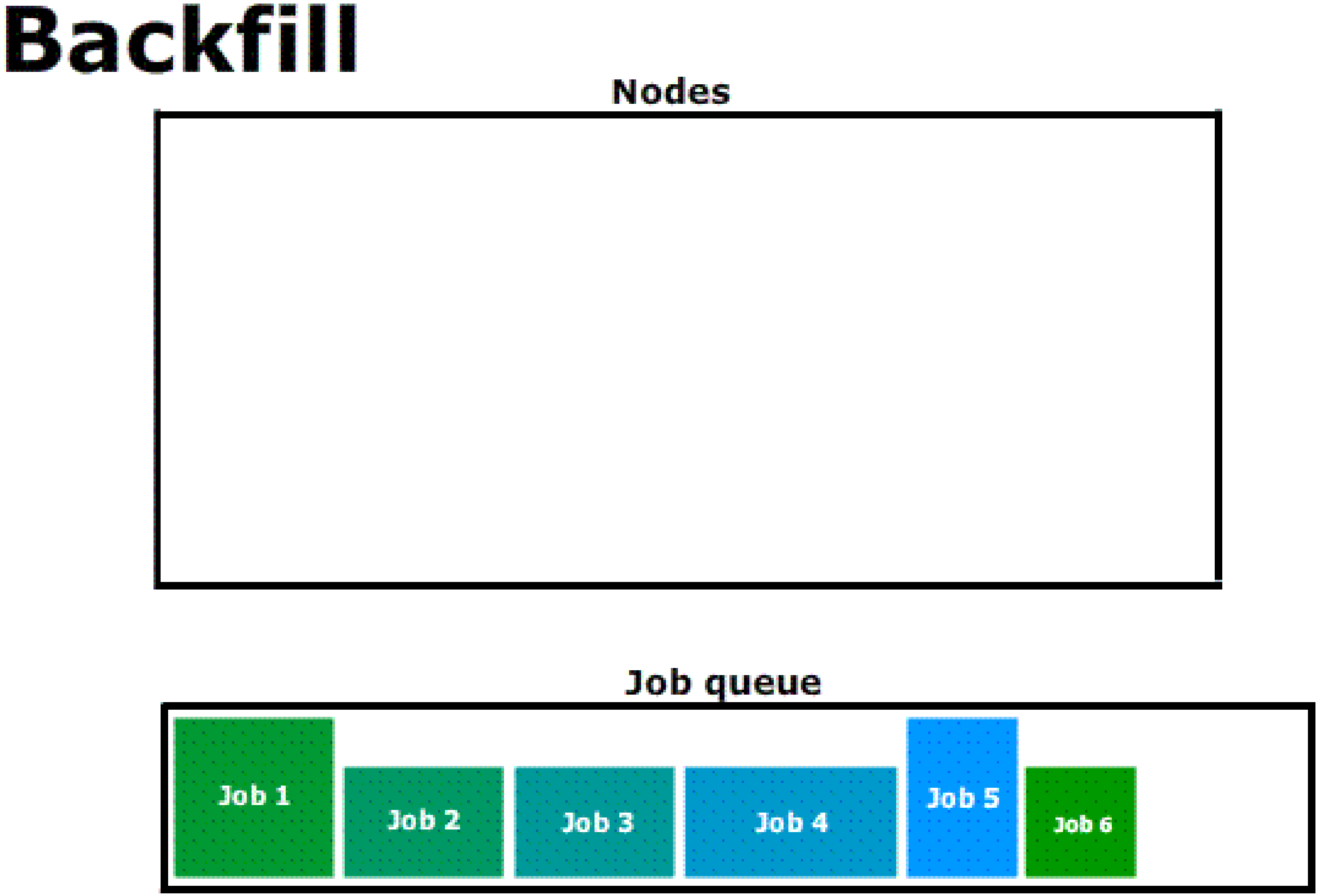
  - `$ qstat` : Get the status of your jobs on the system

- **CPU** nodes: **SINGLE** user policy (only **1 user** per node), Single core jobs can end up on the same node, but are accounted on a job basis.

Job Scheduler: Moab

- The job scheduler decides when and where to run jobs using a priority queue
  - Queries resource manager for runnable jobs
  - Priority is determined by:
    - static properties: credentials, QoS, job resources
    - dynamic properties: fair share, queue time,
  - Tries to optimize resource usage and
    - favors **parallel jobs**,
    - **fair use** of resources for all users (taking into account computation during past 7 days),
    - ensures liveliness, regardless of starting priority, job will eventually have highest priority
    - Small jobs - **backfill**
  - Orders resource manager to start (or stop …) jobs
  - Max queueable jobs per user (100 small, 25/10 big)

Job Scheduler: Moab



Job Scheduler: Moab

- Some Moab commands:
  - `$ checkjob <job-id>` : shows job information
  - `$ showstart <job-id>` : shows the ***earliest*** time job *can, not will* start (at the time of the query)

Understanding Showstart

```
 $ showstart 50036840

INFO:  cannot determine start time for job 50036840

$ showstart 50036840
job 50036840 requires 360 procs for 00:15:00

Estimated Rsv based start in               00:01:00 on Fri Nov 16 12:27:32
Estimated Rsv based completion in          00:16:00 on Fri Nov 16 12:42:32

Best Partition: pbs
```

Understanding checkjob

- `$ checkjob <job-id>` : shows job information

```
job   50029503

AName: my-test
State: BatchHold
Creds: default_project  class:q72h  qos:normal
WallTime:   00:00:00 of 3:00:00:00
BecameEligible: Mon Oct 29 19:11:13
SubmitTime: Mon Oct 29 16:56:04
  (Time Queued  Total: 22:10:10  Eligible: 19:56:00)

Job Templates: 72hour
TemplateSets:  DEFAULT,72hour.set
NodeMatchPolicy: EXACTNODE
Total Requested Tasks: 36

Req[0]  TaskCount: 36  Partition: pbs
Memory >= 5120M  Disk >= 0  Swap >= 0
Dedicated Resources Per Task: PROCS: 1  MEM: 
5120M
NodeSet=ONEOF:FEATURE:[NONE]

Allocated Nodes:
[r22i13n10:36]
Applied Nodeset: r22i13
```

```
SystemID:   Moab
SystemJID:  50031650
Notification Events: JobFail

IWD:
/ddn1/vol1/site_scratch/leuven/304/vsc30468/TEST
Partition List: pbs
Flags:          RESTARTABLE,FSVIOLATION
Attr:           FSVIOLATION,checkpoint,72hour.set
StartPriority:  -3294
IterationJobRank: 0
Holds:          Batch:CannotDebitAccount
 NOTE:  job cannot run  (job has hold in place)
```

Problem with the project = no (not enough) credits available

Understanding Checkjob

```
$ checkjob 50036840
Req[0]  TaskCount: 1  Partition: thinking
Memory >= 2400M  Disk >= 0  Swap >= 0
Dedicated Resources Per Task: PROCS: 1  MEM: 4096M
NodeSet=ONEOF:FEATURE:[NONE]

SystemID:   Moab
SystemJID: 20280125
Notification Events: JobFail

Partition List: thinking
Flags:          RESTARTABLE
Attr:          checkpoint
StartPriority:  1977
Holds:          System:CannotDebitAccount
 NOTE:  job cannot run  (job has hold in place)
```

Just a notification, nothing to be worried about

Problem with the project = no (not enough) credits available

Understanding Checkjob

```
$ checkjob 50036840
Req[0]  TaskCount: 20  Partition: thinking
Memory >= 2400M  Disk >= 0  Swap >= 0
Opsys: ---  Arch: ---  Features: haswell
Dedicated Resources Per Task: PROCS: 1  MEM: 2400M
NodeSet=ONEOF:FEATURE:[NONE]

Allocated Nodes:
[r4i2n6:20]
SystemID:   Moab
SystemJID:  20292673
Notification Events: JobFail  Notification Address: my.name@kuleuven.be

StartCount:     1
Partition List: thinking
Flags:          RESTARTABLE
```

Notification is personalized

```
#PBS -m abe
#PBS -M my.name@kuleuven.be
```

Moab Allocation Manager

$$\#credits = (\boxed{0.000278\cdot walltime}\#nodes)\cdot f_{type}$$

1/3600

Project credits valid for all Tier-2 clusters:

- ThinKing,
- GPU,
- Genius,
- Superdome

$$f_{type} = \begin{cases} 4.76 & \text{ThinKing IvyBridge} \\ 6.68 & \text{ThinKing Haswell} \\ 2.86 & \text{ThinKing GPU} \\ 0 & \text{Superdome} \\ 10 & \text{Genius Thin node} \\ 12 & \text{Genius large memory} \\ 20 & \text{Genius GPU (full node 4xP100)} \\ 5 & \text{Genius GPU 1/4 (1xP100)} \end{cases}$$

Example: `-l walltime=1:00:00 -l nodes=1:ppn=1`

$$\#credits = (0.000278\cdot 3600\cdot 1)\cdot 10 = 10.01$$

`-l walltime=1:00:00 -l nodes=1:ppn=36`

$$\#credits = (0.000278\cdot 3600\cdot 1)\cdot 10 = 10.01$$

Single user per node policy

Credits

Credits card concept:

- Preauthorization: holding the balance as unavailable until the merchant clears the transaction
- Balance to be held as unavailable: based on requested resourced (walltime, nodes)
- Actual charge based on what was really used: used walltime (you pay only what you use, e.g. when job crashes)
- See output file

How to check available credits?

```
$ mam-balance
```

How to check the cost of job?

```
$ module load accounting
$ gquote …
```

Types of queues and default values and limits

- To obtain more detailed information on the queues

$ **qstat -f -Q <queuename>**

- **`qstat -f -Q q1h`**

```
Queue: q1h
    queue_type = Execution
    max_user_queuable = 200
    total_jobs = 37
    state_count = Transit:0 Queued:21 Held:0 Waiting:0 Running:0 Exiting:0 Com
        plete:16
    resources_max.walltime = 01:00:00
    resources_min.walltime = 00:00:01
    resources_default.nodes = 1:ppn=36
    resources_default.partition = pbs
    resources_default.pmem = 5gb
    resources_default.walltime = 01:00:00
    mtime = 1540971884
    resources_assigned.nodect = 0
    resources_assigned.mem = 0b
    enabled = True
    started = True
```

Software

modules

Software: Genius

- Operating system
  - CentOS 7.4.1708, 64 bit
  - Kernel 3.10.0-693.17.1.el7.x86_64
- Applications
- For development
  - Compilers & basic libraries ≡ tool chains
  - Libraries
  - Tools: debuggers, profilers

Different on each cluster!

Use modules

If no module is loaded:

You can use only software available on the basic CentOS Linux: older versions of software, without extensions

Available tool chains

	intel tool chain	foss tool chain
Name	intel	foss
version	2018a	2018a
Compilers	Intel compilers (v 2018.1.163) icc, icpc, ifort	GNU compilers (v 6.4.0-2.28) gcc, g++, gfortran
MPI Library	Intel MPI	OpenMPI
Math libraries	Intel MKL	OpenBLAS, LAPACK FFTW ScaLAPACK

***Tool chain**:* set of programming tools to build an application

Never mix different toolchains!

Modules

Set the environment to use software package:

- `$ module available` or `module available Py`
  - Lists all installed software packages
- `$ module av |& grep -i python`
  - To show only the modules that have the string 'python' in their name, regardless of the case
- `$ module load Python/2.7.14-foss-2018a`
  - Adds the ‘matlab’ command in your PATH
- `$ module load GCC`
  - ‘Load’ the (default) GCC version – not recommended, not reproducible
- `$ module list`
  - Lists all ‘loaded’ modules in current session
- `$ module unload Python/2.7.14-foss-2018a`
  - Removes all only the selected module, other loaded modules – dependencies are still loaded
- `$ module purge`
  - Removes all loaded modules from your environment

Modules

- `$ module swap foss intel`
  - = module unload foss; module load intel
- `$ module try-load packageXYZ`
  - try to load a module with no error message if it does not exist
- `$ module keyword word1 word2 ...`
  - Keyword searching tool, searches any help message or whatis description for the word(s) given on the command line
- `$ module help foss`
  - Prints help message from modulefile
- `$ module spider foss`
  - Describes the module

Modules: Genius

- **ml** – convenient tool
- `$ ml`
  - = module list
- `$ ml foss`
  - =module load foss
- `$ ml -foss`
  - =module unload foss (not purge!)
- `$ ml show foss`
  - Info about the module

More info: http://lmod.readthedocs.io/en/latest/010_user.html

Get started

Prices

Introduction credits

- Maximum 2000
- Valid up to 6 months

FREE

Project credits

- Commercial partner **0.06 €**
- Internal funding, IWT, FWO, European funding **0.0035 €**
- Minimum purchase 5000 credits

Storage

- /scratch, temporary quota upgrade FREE
- /data 25 GB , 14.63 €/year
- HPC archive 1 TB, 70 €/year
- /staging 1 TB, 130 €/year

Application support

- Software Installation
- Debugging & profiling up to 5 days
- Parallelization & optimization up to 5 days

FREE

Training

- Scheduled courses
- Infosessions
- Thematic workshops

FREE

Prices and information: https://icts.kuleuven.be/sc/english/HPC

Extra services

- Request introduction credits
  https://admin.kuleuven.be/icts/onderzoek/hpc/request-introduction-credits
- Request project credits
  https://admin.kuleuven.be/icts/onderzoek/hpc/request-project-credits

  https://icts.kuleuven.be/sc/forms/Aanvraagformulier_HPC_Credits
- Extra project credits (to add to existing project)

  https://admin.kuleuven.be/icts/onderzoek/hpc/extra-project-credits
- Request extra storage

  https://admin.kuleuven.be/icts/onderzoek/hpc/hpc-storage

Job types

1) **Batch jobs** are by far the most common, and allow for the most efficient use of the infrastructure. Essentially, a batch job is a bash shell script that is executed on a compute node, and that can spawn a parallel computation on many nodes. These jobs are placed in the queue, and the user can forget about it until it is finished.
2) **Interactive jobs** are intended to work on one or more compute nodes interactively. This can be useful in the context of software development for debugging and profiling applications, or for interactive calculations or visualizations. Basically, one gets a shell on one of the compute nodes.
3) To get GPU(s), you can use **JupyterHub** with your internet browser

Glossary

- **Walltime**: the actual time an application runs (as in clock on the wall), or is expected to run. When submitting a job, the walltime refers to the maximum amount of time the application can run. For accounting purposes, the walltime is the amount of time the application actually ran, typically less than the requested walltime.
- **Memory requirement**: the amount of RAM needed to successfully run an application. It can be specified per process for a distributed application, expressed in GB.
- **Storage requirement**: the amount of disk space needed to store the input and output of an application, expressed in GB or TB.

Interactive jobs

- `$ qsub -I -A lp_hpcinfo_training`
  - opens shell on a compute node for 1h
- `$ qsub -I -X -A lp_hpcinfo_training`
  - opens shell, with X-forwarding
- `$ qsub -I -l nodes=2:ppn=36,walltime=8:00:00 -A lp_hpcinfo_training`
  - open shell for 8h, with access to 2 nodes, 36 cores each

ppn: number of cores

Time of the job execution of the cluster

Simple batch job

- Contents of file `myjob.pbs` (a PBS job script, actually bash):

```
#!/bin/bash -l
echo Hello World
```

- To run job, enter

```
$ qsub myjob.pbs -A lp_hpcinfo_training
  50009076. tier2-p-moab-2.tier2.hpc.kuleuven.be
```

  Result

```
$ ls
myjob.pbs
myjob.pbs.e500009076
myjob.pbs.o500009076
```

Error and output files

- Error file `myjob.pbs.e50009076`
  - Contains any errors that occured during execution
  - Useful to determine why your job failed
  - Always created, if no problems – file is empty

- forrtl: error (78): process killed (SIGTERM)
  Stack trace terminated abnormally.

Programming problem

- =>> PBS: job killed: walltime 432031 exceeded limit 432000

Too short walltime

- IOError: [Errno 122] Disk quota exceeded

Not enough disk space

Error and output files

- Output file `myjob.pbs.o50009076`
  - Contains output to standard output
  - Info about requested resources and used resources

```
time: 900
nodes: 1
procs: 1
account string:
lp_hpcinfo_training
queue: q1h
```

Error and output files

- Output file `myjob.pbs.o50132389`

```
Allocated nodes:
r05i01n16
Job ID: 50132389. tier2-p-moab-2.tier2.hpc.kuleuven.be
User ID: vsc30468
Group ID: vsc30468
Job Name: cmeAMRnew.sh
Session ID: 52711
Resource List: neednodes=1:ppn=1,nodes=1:ppn=1,pmem=1gb,walltime=00:15:00
Resources Used: cput=00:00:36,mem=937748kb,vmem=1472672kb,walltime=00:00:37
Queue Name: q1h
Account String: lp_hpcinfo_training
-------------------------------------------------------------------------------
time: 37
nodes: 1
procs: 1
account: lp_sys
```

Batch job with resource specifications

- From command line

```
$ qsub -l walltime=10:00:00 myjob.pbs
```

- In a PBS job script

```
#!/bin/bash -l
#PBS -l walltime=10:00:00
#PBS -l nodes=2:ppn=36
#PBS -l pmem=5200mb
#PBS -N myjob2
#PBS -A default_project
#PBS -o $PBS_JOBID.stdout
#PBS -e $PBS_JOBID.stderr
#PBS -m ae
#PBS -M my.name@kuleuven.be
```

If not specified:
walltime=01:00:00

If not specified:
nodes=1:ppn=1

If not specified:
pmem=5gb

If not specified: job will not start

- default_project = intro credits
- lp_my_project_= project credits
- lp_hpcinfo_training = project credits for the course exercises

Capture standard output and error during at runtime

My first pbs script

```
#!/bin/bash -l
#PBS -l walltime=00:30:00
#PBS -l nodes=1:ppn=36
#PBS -N testjob
#PBS -A lp_hpcinfo_training
#PBS -m abe
#PBS -M my-name@kuleuven.be

module purge
module load matlab/R2018a

cd $VSC_SCRATCH
cd $PBS_O_WORKDIR

matlab -nojvm -nodisplay -r mat
```

~~exit 0~~

Clean the modules loaded by default in .bashrc
Load all the necessary modules (new shell is started for each job)

Go to the directory where your code and input files are located
$PBS_O_WORKDIR= location from which the job was submitted

Execute the code

Do not add unnecessary statements – in case of problem real exit code is overwritten, finding source of problem may be impossible

Using GPU(s)

- On Genius, you can request a fraction of a node with 1, 2, 3 or 4 GPUs.
- Then, you will be granted a fraction of cores and memory, too.
- E.g.

```
$> qsub -l partition=gpu,nodes=1:ppn=9:gpus=1      1 GPU
$> qsub -l partition=gpu,nodes=1:ppn=18:gpus=2     2 GPUs
$> qsub -l partition=gpu,nodes=1:ppn=27:gpus=3     3 GPUs
$> qsub -l partition=gpu,nodes=1:ppn=36:gpus=4     Full Node
```

Remarks

- Different users may use the same node
- Note: `pmem=5gb` is still OK
- You will be debited for credits the same fraction of node costs as you use

PBS Script

```
#!/bin/bash -l
#PBS -l walltime=00:30:00
#PBS -l partition=gpu
#PBS -l nodes=1:ppn=18:gpus=2
#PBS -N testjob
#PBS -A lp_hpcinfo_training
#PBS -m abe
#PBS -M my-name@student.kuleuven.be
```

Large-Memory Jobs

You have two options:

1) Use (10) dedicated large-memory machines on Genius

```
$> qsub -l partition=bigmem,nodes=1:ppn=36,mem=760gb -A
…
```

2) Or use the Superdome machine

```
$> module load superdome
$> qsub -l partition=superdome -q qsuperdome \
        -L tasks=1:lprocs=42:place=numanode=3 -A…
```

PBS Script

```
#!/bin/bash -l
#PBS -l walltime=00:30:00
#PBS -l partition=bigmem
#PBS -l nodes=1:ppn=36
#PBS -l mem=760gb
#PBS -A lp_hpcinfo_training
#PBS -m abe
#PBS -M my-name@student.kuleuven.be
```

Remarks

- `pmem` is memory per process, i.e.
  `pmem = mem / ppn`
- Set either `mem` OR `pmem`
- Always set 4 – 8 GB memory for the operating system

Debugging / Testing Jobs

- Sometimes, you need to test/debug your (parallel) application quickly
- ThinKing and Genius have each **2** dedicated nodes for debugging purposes
- Such jobs do **not** go to the normal queue, so they start faster
- Max. walltime is **30 minutes**
- You must specify Quality of Service (qos)

Request Debugging Nodes

```
$> qsub -l nodes=2:ppn=10 -l partition=gpu -l qos=debugging -l
walltime=30:00 -A lp_hpcinfo_training
```

Managing & Monitoring Jobs

Command	Purpose
`$> qsub ….`	Submit a job (batch/interactive)
`$> qdel <JobID>`	Delete a specific job
`$> checkjob -v -v -v <JobID>`	Very detailed job info (very useful to diagnose issues)
`$> qstat -n`	Status of all recent jobs
`$> qstat -Q -f`	Info about available queues
`$> showstart <JobID>`	Give a *rough* estimate of start time

`$> showq`
`$> showq -p gpu`
	Show minimal info about a queue or partition (`-p`)

`$> pbstop`	Overview of the cluster
`$> mam-balance`	Overview of different credit projects that you can use (`qsub -A <Project>`)
`$> mam-list-allocations`	Detailed overview of your credit projects

How do I acknowledge the VSC in publications?

- Acknowledging the VSC in all relevant publications helps the VSC secure funding, and hence you will benefit from it in the long run as well. It is also a contractual obligation for the VSC.
- If you are in the KU Leuven association, you are also requested to add the relevant papers to the virtual collection "High Performance Computing" in Lirias – it helps to generate the publication lists with relevant publications.
- Please use the following phrase to do so in **Dutch** “*De rekeninfrastructuur en dienstverlening gebruikt in dit werk, werd voorzien door het VSC (Vlaams Supercomputer Centrum), gefinancierd door het FWO en de Vlaamse regering – departement EWI*”,
- or in **English**: “*The computational resources and services used in this work were provided by the VSC (Flemish Supercomputer Center), funded by the Research Foundation - Flanders (FWO) and the Flemish Government – department EWI*”.

Hands-on 2

- Copy /apps/leuven/training/HPC_intro to your $VSC_DATA directory and go to this directory

```
cp -r /apps/leuven/training/HPC_intro $VSC_DATA;
cd $VSC_DATA/HPC_intro
```

- Submit jobscript cpujob.pbs to the cluster

```
qsub cpujob.pbs
```

- Check the status of your job(s) (`qstat`)
- Analyze outputs (i.e. display the output file – commands `cat filename` or `more filename` or `less filename`)

- If you compute other types of jobs – try sas/matlab/mpi job

Questions

- Now
- Helpdesk:
  hpcinfo@kuleuven.be or
  https://admin.kuleuven.be/icts/HPCinfo_form/HPC-info-formulier
- VSC web site:
  http://www.vscentrum.be/
  - VSC documentation: https://vlaams-supercomputing-centrum-vscdocumentation.readthedocs-hosted.com/en/latest/
    VSC agenda: training sessions, events
- Systems status page:
  http://status.kuleuven.be/hpc

While we don't have…

Talk to us!!!

Do not send screenshots – we need to retype all the paths/commands

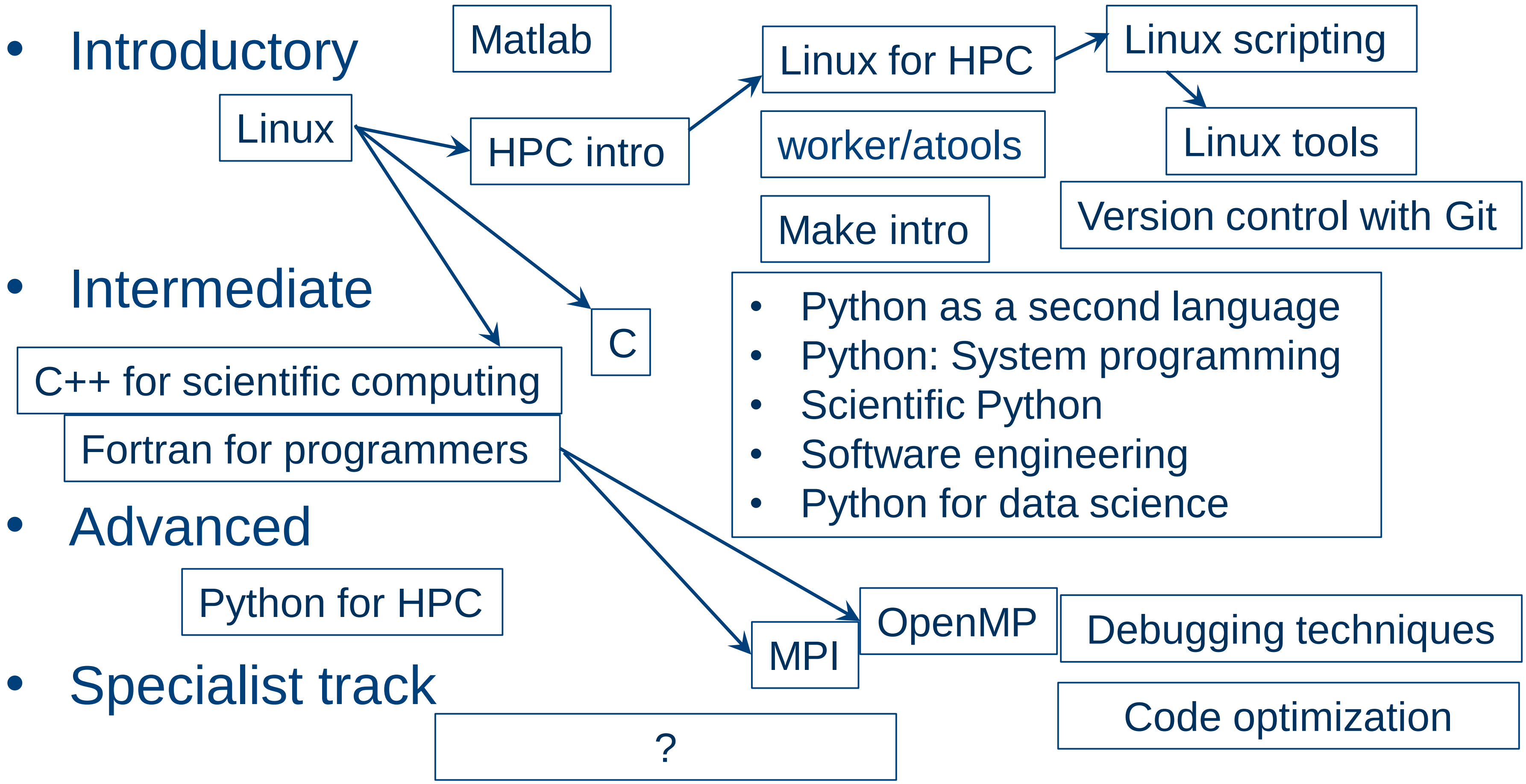
Please send the copied output and all the info:

- vsc id
- job id
- submitted script
- error/output file of the job

VSC training 2019/2020

Info sessions:

- Containers
- Notebooks



- Introductory

Matlab

Linux

HPC intro

Linux for HPC

Linux scripting

Linux tools

worker/atools

Make intro

Version control with Git

- Intermediate

C

C++ for scientific computing

Fortran for programmers

- Python as a second language
- Python: System programming
- Scientific Python
- Software engineering
- Python for data science

- Advanced

Python for HPC

MPI

OpenMP

Debugging techniques

Code optimization

- Specialist track

?

Stay up-to-date https://www.vscentrum.be/training