VSC HPC Introduction

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Questions and problems troubleshooting

- Blackboard Collaborate session: https://eu.bbcollab.com/guest/ce4229a2f9eb4cc5b90f490d660eb1c2

Material

- ❑ Everything is on Github: https://hpcleuven.github.io/HPC-intro/
- ❑ Video Recordings
  - Scan the QR code
  - Recommended videos: ~ 2 hrs
  - Optional videos: ~1 hr

What is High Performance Computing?

- using supercomputers to solve advanced computation problems
- Reduce the computation time from days, years, decades, or centuries to minutes, hours, days, or weeks
- The key is parallelism

In practice, it is more like …

The concept is simple: **Parallelism** = employing multiple processors for a single problem

Outline

- What is the VSC?
- What is a cluster?
- Genius Cluster
- Storage
- Login nodes
- Connection Setup
- Software environment
- How to submit jobs?
- Dedicated hardware
- How to choose resources?
- Optional material
  - Linux in brief
  - Conda for Python and R
  - Worker Framework

VSC

(Vlaams Supercomputer Centrum)

VSC PARTNERSHIP

Supported by

fwo

ASSOCIATIE UNIVERSITEIT GENT

universitaire associatie BRUSSEL

ASSOCIATIE KU LEUVEN

antwerp university association

ASSOCIATIE UNIVERSITEIT-HOGESCHOLEN LIMBURG

VSC HPC Environments

Tier-0

PRACE

Vlaanderen
is supercomputing

Tier-1

BrENIAC

Tier-2

GHENT UNIVERSITY — STEVIN

VUB VRIJE UNIVERSITEIT BRUSSEL — HYDRA

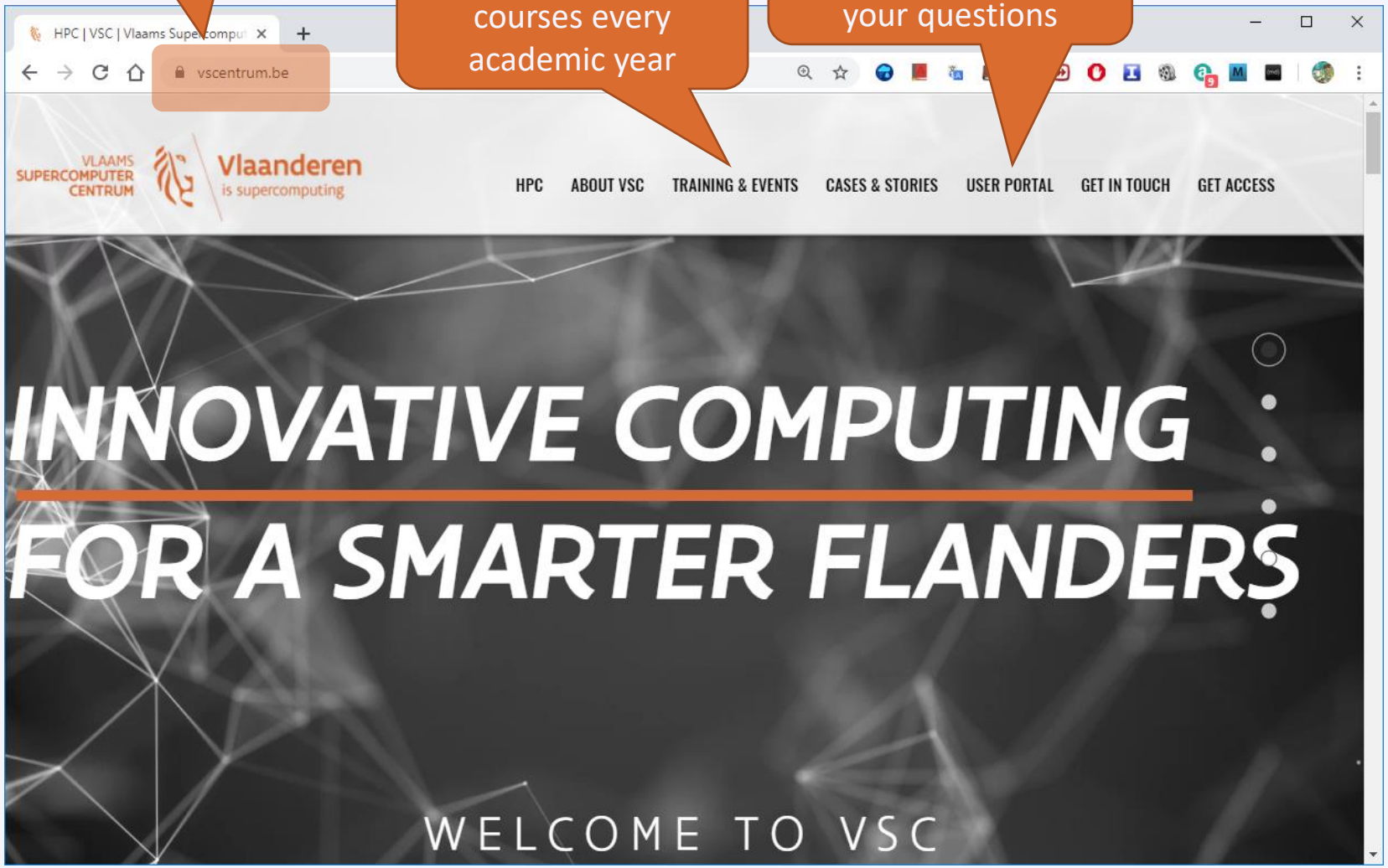
Universiteit Antwerpen — HOPPER/LEIBNIZ

KU LEUVEN UHASSELT — THINKING//GENIUS

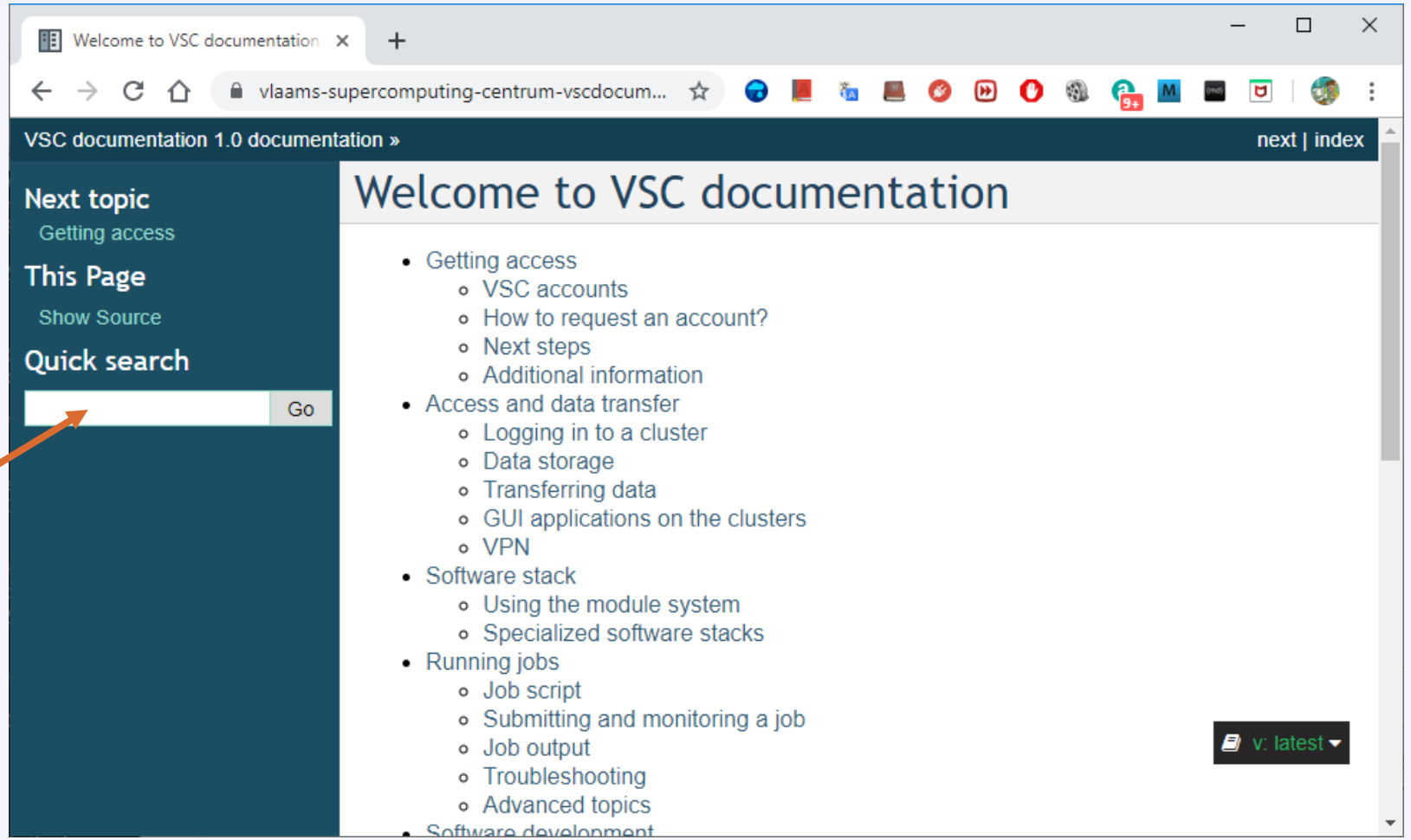
www.vscentrum.be

Very rich suite of courses every academic year

Documentation! Answers >80% of your questions



VLAAMS SUPERCOMPUTER CENTRUM

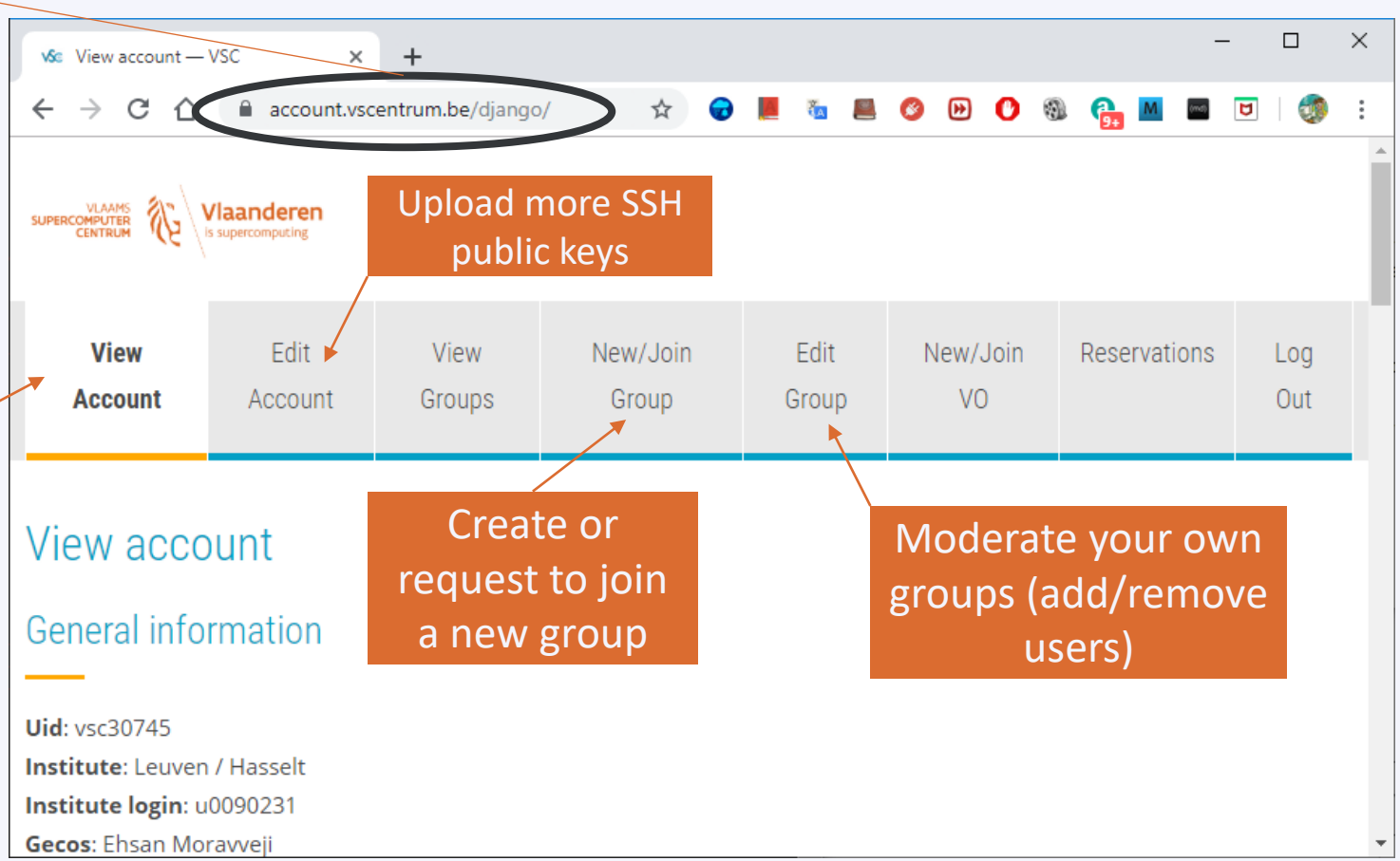


Search you keywords here; e.g. qsub

Support and Services

Basic support	• Helpdesk (hpcinfo@kuleuven.be) • Monitoring and reporting
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

To manage your VSC account: account.vscentrum.be



Upload SSH Key
Request account

Create or request to join a new group

Moderate your own groups (add/remove users)

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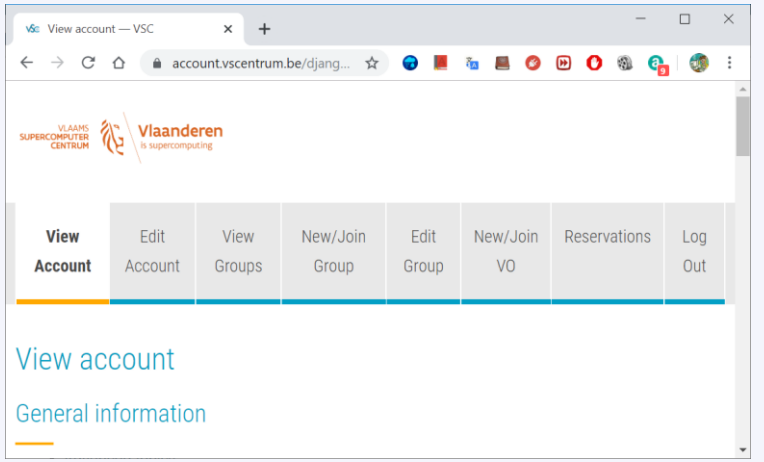
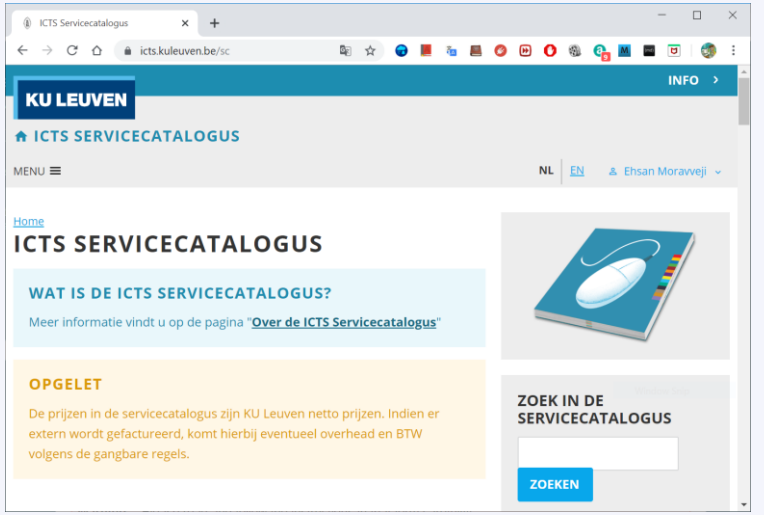
Become a VSC user

- ❑ Create a secure (4096 bit) SSH key pairs
  Upload it on the account page: www.account.vscentrum.be
- ❑ You need to request a VSC account
  Normally processed swiftly
- ❑ Request introductory credits (2000 free credits for 6 months)
- ❑ Request project credits (for supervisors and project leaders)
  You need to create a VSC group
  Add users to the group to give them access to use credits
  Fill out the request form
- ❑ Extra storage requests
  Scratch extension: free of charge
  Archive fileset: 70 € per TB per year
  Staging fileset: 130 € per TB per year
- ❑ All service costs (compute and storage) are all explained
  Go to ICTS service catalogus: https://icts.kuleuven.be/sc
  Click on High Performance Computing (NL/EN)





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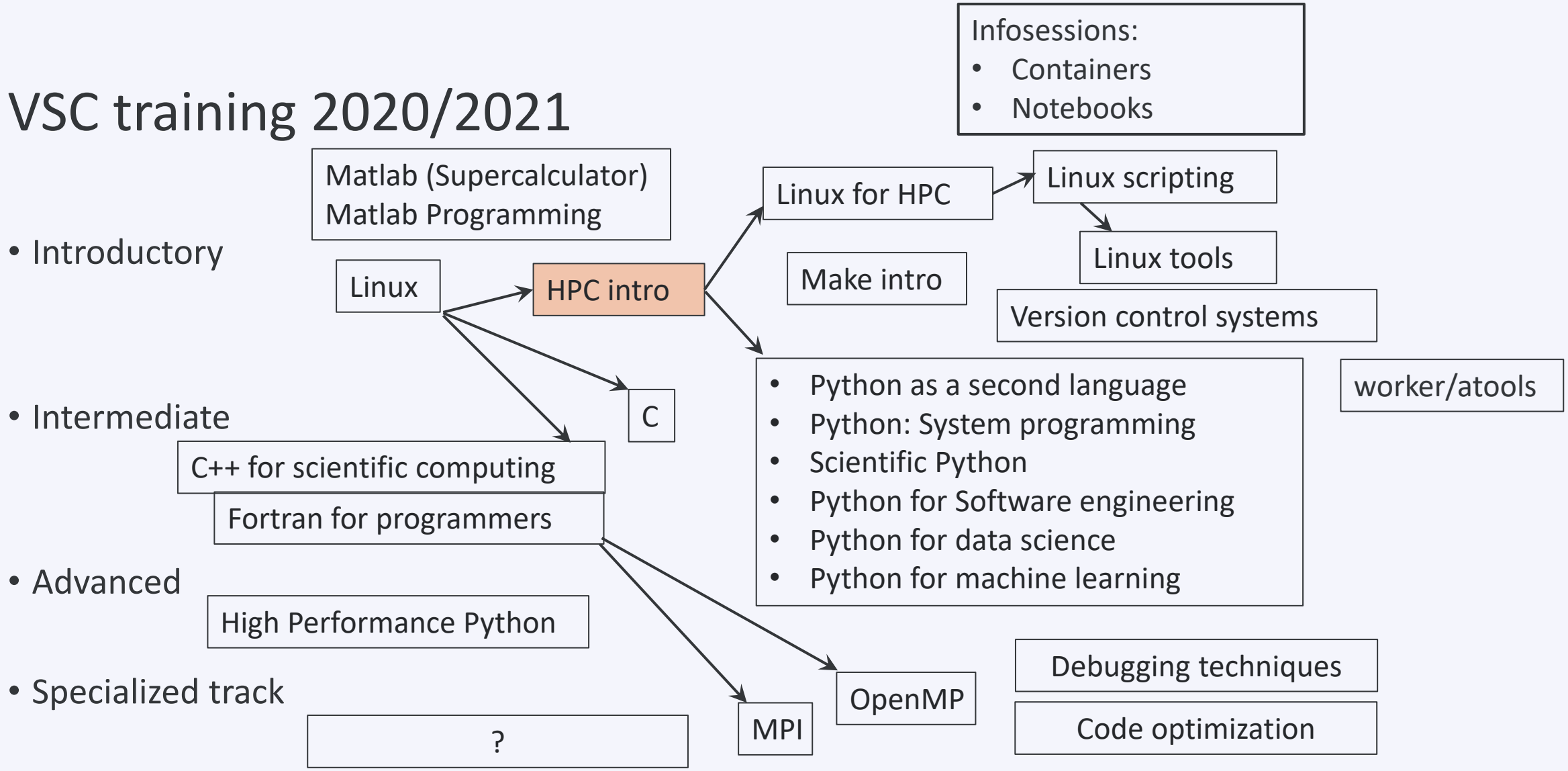
VSC training 2020/2021



PRACE MOOC Defensive programming and debugging: https://www.futurelearn.com/courses/defensive-programming-and-debugging

To Acknowledge VSC in publications

Why?

- ❑ a contractual obligation for the VSC
- ❑ helps VSC secure funding
- ❑ you will benefit from it in the long run

At KU Leuven

- ❑ add the relevant papers to the virtual collection "High Performance Computing" in Lirias

In het nederlands

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.

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.

Tier-2 Clusters

Tier-2 Clusters @ KU Leuven

ThinKing (since 2014)
352 nodes: 7,616 cores

Genius (since 2018)
250 nodes: 8,936 cores

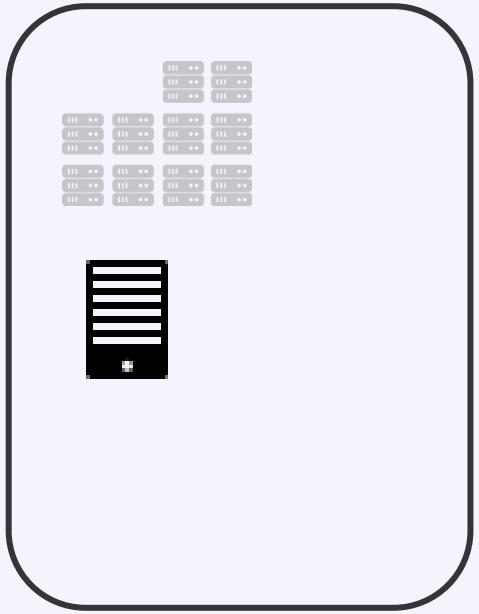
Tier-2 Overview

Compute nodes

Thinking:
+ 48x + 86x Haswells 24c 64/128 GB

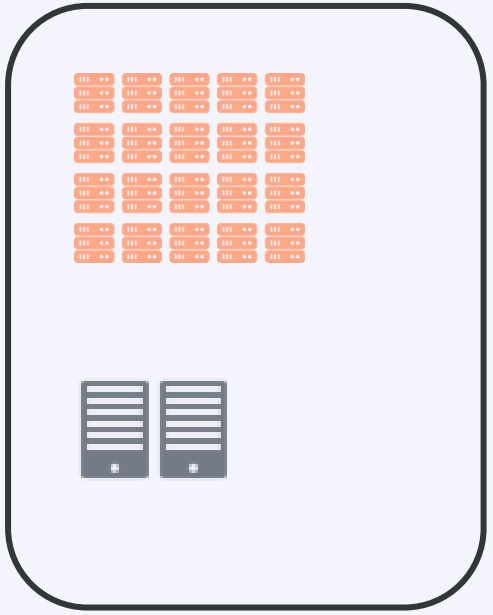
Genius:
+ 96x Skylake 36c 192 GB
+ 144x CascadeLake 36c 192 GB

Large memory nodes



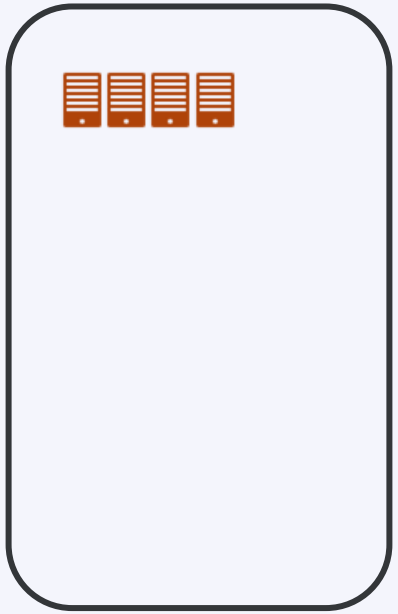
Genius:
+ 10x Skylake 36c 768GB
+ 1x Superdome 112c 6 TB

GPU nodes



Genius:
+ 20x Skylake 36c 192 GB
  4x P100 16GB
+ 2x CascadeLake 36c 768GB
  8x V100 32GB

Exp nodes



Genius:
4 AMD Naples 64c 256 GB

Technical Hardware Specifications

	Tier 2					Tier 1		
Cluster name	ThinKing		Genius			BrENIAC		
Processor type	Haswell		SkyLake		Cascade Lake	Broadwell		SkyLake
Cores per node	24		36		36	28		28
Base Clock Speed	2.5 GHz		2.3 GHz		2.6 GHz	2.4 GHz		2.6Ghz
Total nodes	48	96	86	10	144	580		408
Node memory (GB)	64	96	192	768	192	128	256	192
Memory per core (GB)	2.5	3.8	5.2	21.2	5.3	4.4	9.0	6.7
Total cores	3,456		3,456		4,320	27,664		
Peak performance (Flops/cycle)	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		16 DP FLOPs/cycle: 8-wide FMA (fused multiply-add) instructions AVX-512	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
Network	Infiniband FDR		Infiniband EDR		Infiniband EDR	Infiniband EDR		
Cache (L1 KB/L2 KB/L3 MB)	12x(32i+32d) / 12x256 / 30MB		18x(32i+32d) / 18x1024 / 25 MB		18x(32i+32d) / 18x1024 / 25 MB	14x(32i+32d) / 14x 256 / 35 MB		18x(32i+32d) / 18x1024 / 25 MB

Genius

SkyLake (since 8/2018)
CascadeLake (since 1/2020)

Tier-2 Cluster: Genius

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**
CascadeLake	Gold 6240	IB-EDR	**36**	**192 GB**	800 GB	**144**
CascadeLake **GPU**	Gold 6240 **8xV100** SMX2	IB-EDR	**36**	**768 GB**	800 GB	**2**
SkyLake **Superdome**	Gold 6132	Flex Grid	**14**	**6 TB**	6 TB	**8**

Storage

Overview of the storage infrastructure

- Your files are owned only by you.
  Other VSC users have no permission to read/write/execute your files (POSIX)
- A VSC account has 3 default storages (free of charge)
  - `$VSC_HOME`
  - `$VSC_DATA`
  - `$VSC_SCRATCH`
- You can additionally request `staging` and `archive` storages
- Different storage volumes have different:
  - mount point
  - size and performance
  - use case
  - backup and maintenance policy
- More info on ICTS Service Catalog (EN/NL)

Storage

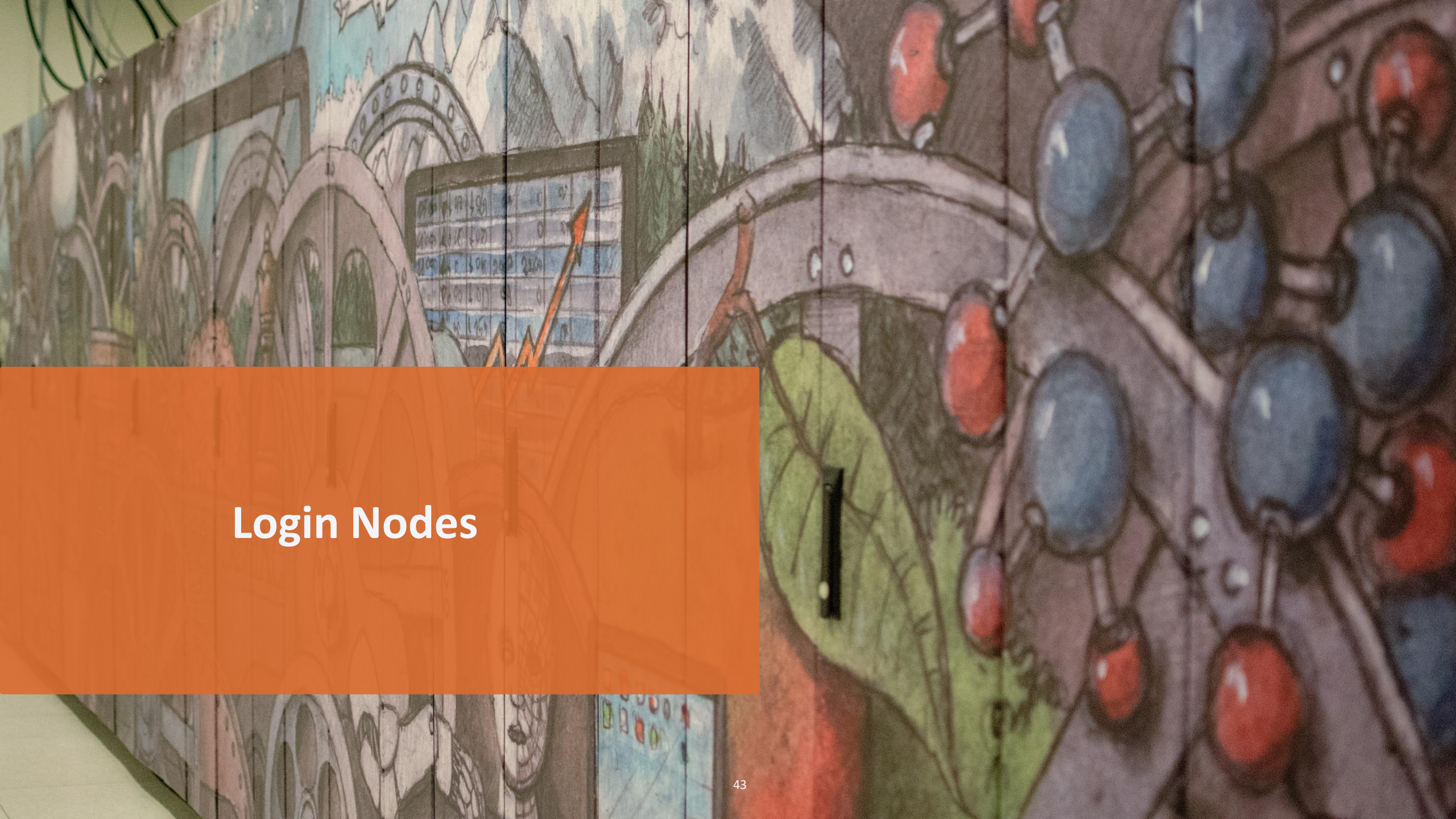
- Request form for extra storage
- More information
- Do not use `/tmp`
  It is only 10 GB and is reserved for the OS and root processes
  Your application can crash if using `/tmp`
- You are automatically logged into your home folder upon login.
  Make sure you immediately go to your other storages, e.g.
  `$ cd $VSC_DATA`
- Always check your storage balance using `myquota` command

Example

```
$ myquota
file system $VSC_HOME
    Blocks: 1479M of 3072M
    Files: 12934 of 100k
file system $VSC_DATA
    Blocks: 102G of 225G
    Files: 1043k of 10000k
file system $VSC_SCRATCH
    Blocks: 15M of 1.5T
```

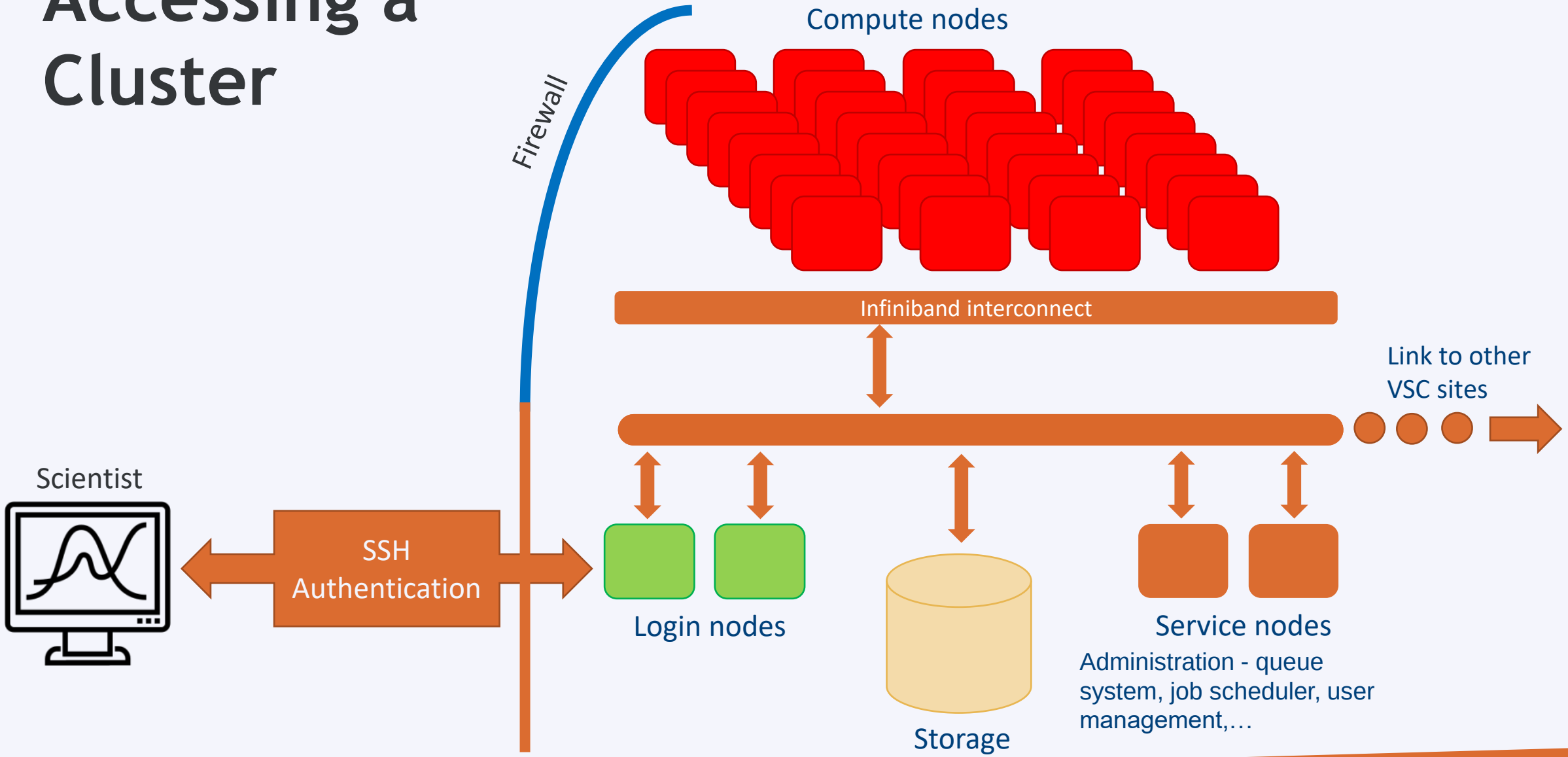
Storage Areas

Env. Variable	$VSC_HOME	$VSC_DATA	$VSC_SCRATCH
Full Path	/usr/leuven/3XX/vsc3XXXX	/data/leuven/3XX/vsc3XXXX	/scratch/leuven/3XX/vsc3XXXX
Filesystem Type	NFS	NFS	Lustre
Access	Global	Global	Global
Backup	Yes (hourly/daily/weekly)	Yes (hourly/daily/weekly)	No files are deleted 28 days after last access
Quota	3 GB	75 GB	100 GB
Extension	No	paid	free
Use Case	Storing SSH key & config files	Install software, keep codes and data for longer term	Intensive I/O, temporary storage



Login Nodes

Accessing a Cluster



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Using Login Nodes

Tips

- ❑ To develop and/or compile code and/or software
- ❑ To check your storage and credit balance
- ❑ To manage jobs (submit, check status, debug, resubmit, …)
- ❑ To move data around
  within VSC: use data, scratch, staging, archive
  outside VSC: copy/sync from/to your local storage
- ❑ To pre-process or post-process your data/jobs
- ❑ To visualize your data
- ❑ To share files/folders

Warning

- ❑ Login nodes are shared resources
- ❑ **Do not** execute heavy-lifting tasks (core, memory)
- ❑ Instead, submit jobs

Login Hosts on Different Machines/partitions

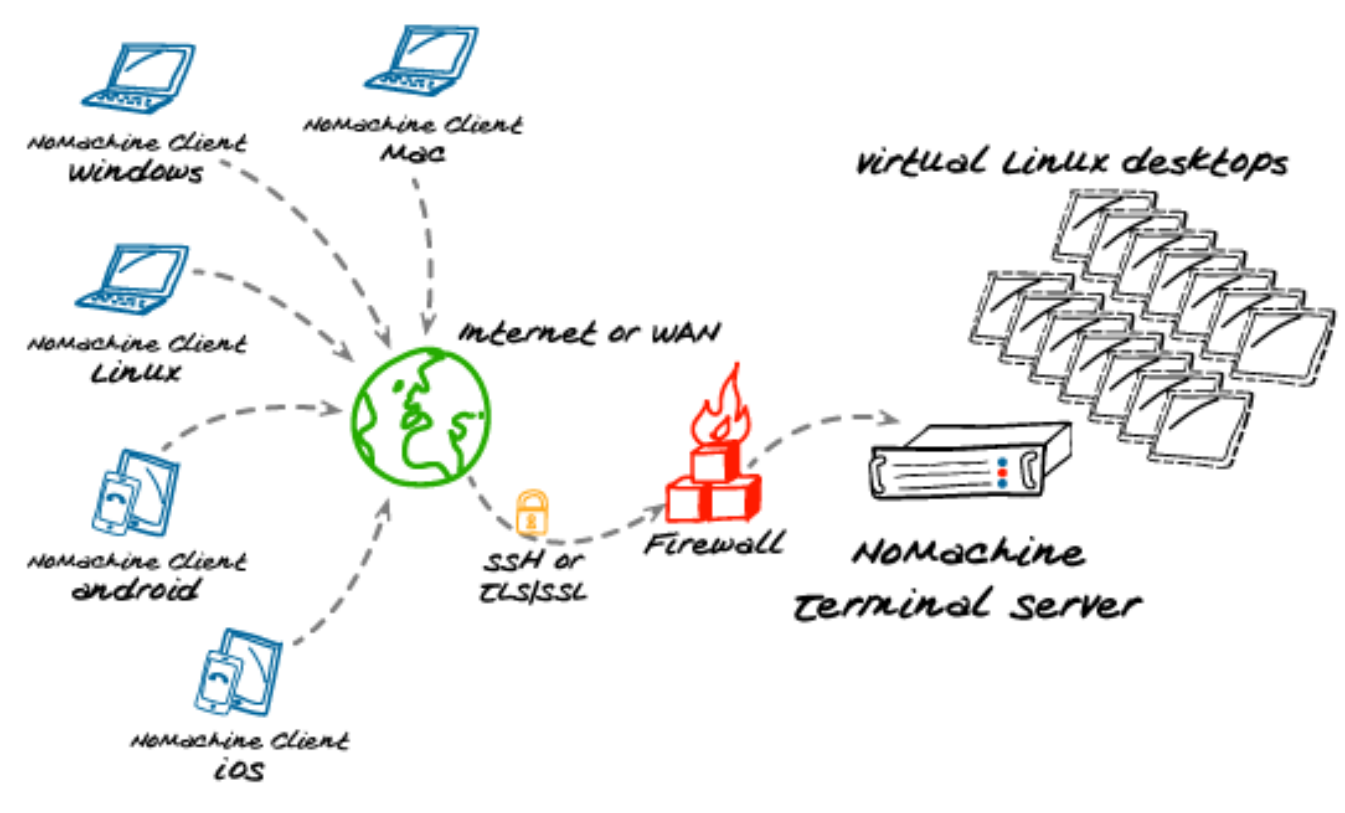
- Windows: PuTTY or MobaXterm or NX
  Linux/Mac: terminal or NX
- To login, you need an active VSC number and a hostname
  `$ ssh -X vscXXXXX@<hostname>`

Cluster / Partition	<hostname>	Remark(s)
ThinKing	`login-thinking.hpc.kuleuven.be`	Recommended
	`login7-tier2.hpc.kuleuven.be` `login8-tier2.hpc.kuleuven.be`	Haswell partition
Genius	**`login.hpc.kuleuven.be`** `login-genius.hpc.kuleuven.be`	Recommended
	`login{1,2}-tier2.hpc.kuleuven.be`	No GPU
	`login{3,4}-tier2.hpc.kuleuven.be`	Nvidia Quadro P6000

NX – The Graphical Login

NX is:

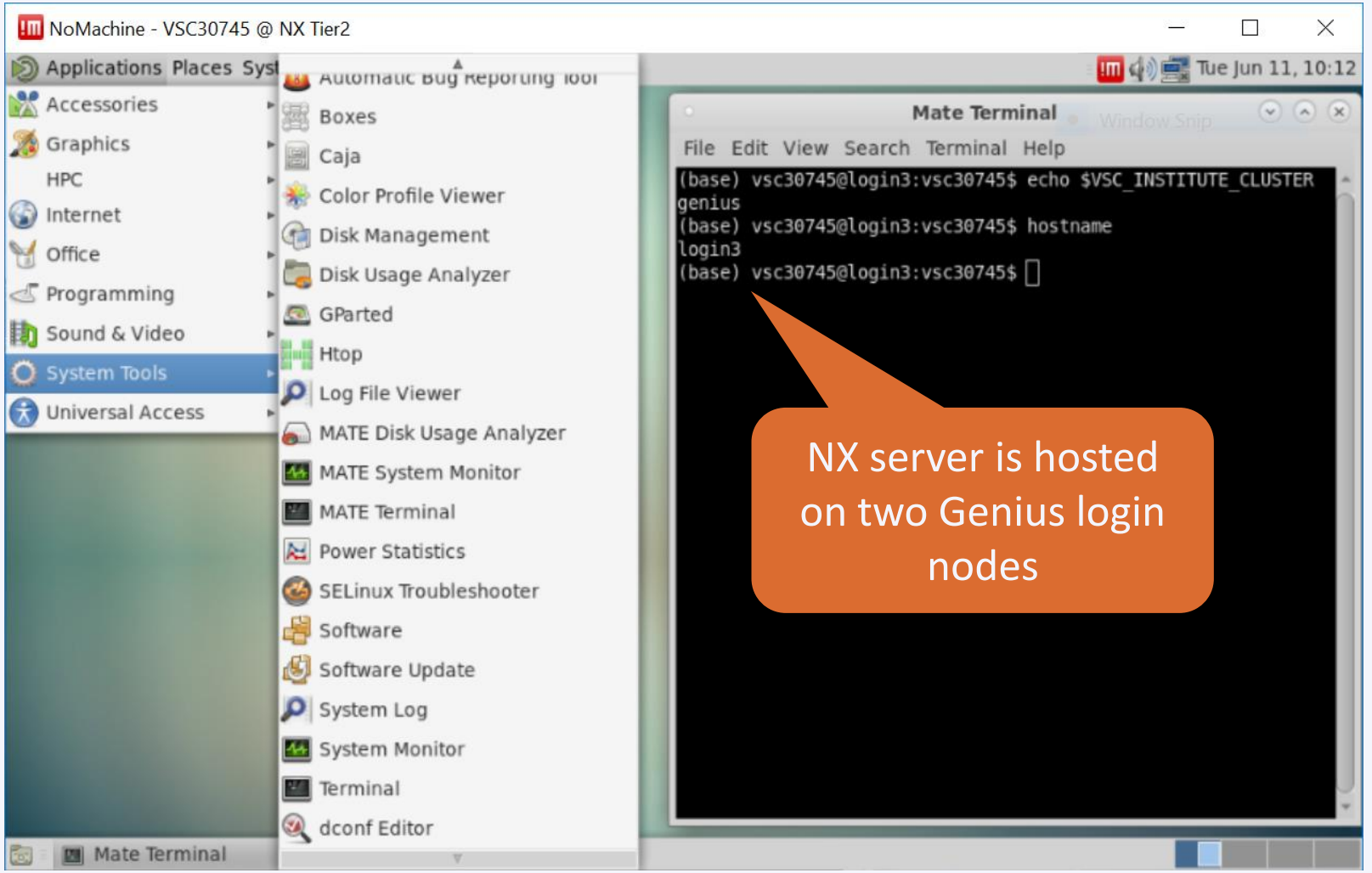
- ❑ a graphical remote desktop server
- ❑ login to VSC
- ❑ start a virtual Linux instance(s)
- ❑ Client: NoMachine
- ❑ Configuration Guide
- ❑ Using OpenSSH key
  Convert your key



Advantages of NX

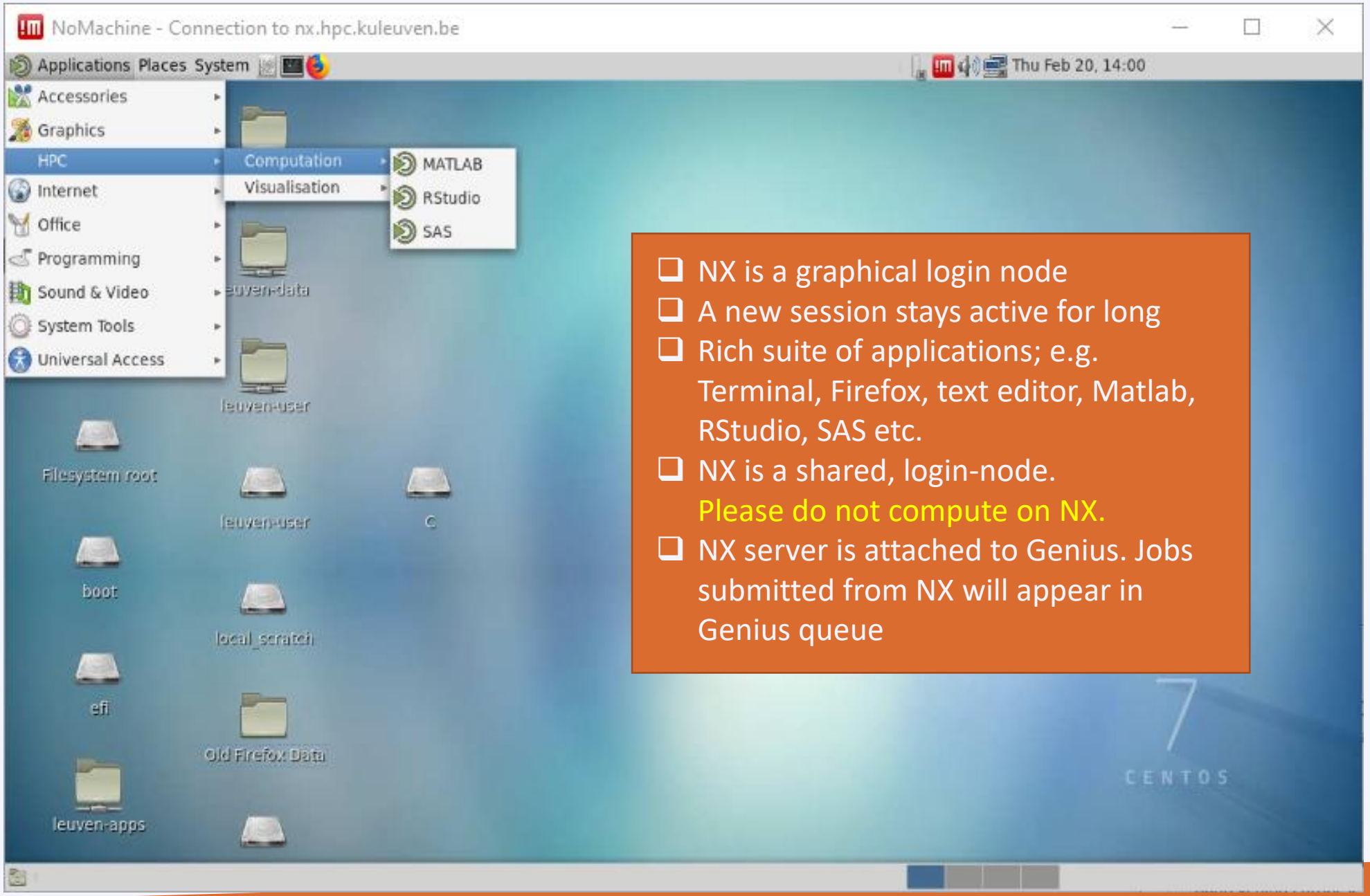
- ❑ Graphical login
- ❑ A session stays alive/active even if you close your client (e.g. laptop)
- ❑ Resume a session, and immediately keep working where you left off
- ❑ More interactive jobs
- ❑ Available apps:
  - Internet browser, terminal, …
  - Text editor, PDF reader, Image viewer, …
  - Matlab, RStudio, SAS
- ❑ Remark:
  - NX is shared among tens of users
  - **Do not compute/test your code there**
  - Instead, submit jobs from NX to compute nodes

NX virtual desktop



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 though modules from Terminal.



- NX is a graphical login node
- A new session stays active for long
- Rich suite of applications; e.g. Terminal, Firefox, text editor, Matlab, RStudio, SAS etc.
- NX is a shared, login-node. Please do not compute on NX.
- NX server is attached to Genius. Jobs submitted from NX will appear in Genius queue

Software Stack

Software: Available Modules

- OS: Linux CentOS 7.7, Kernel 3.10.0-1127.18.2.el7.x86_64
- Toolchains:
  Intel 2018a (icc, icpc, ifort; Intel MPI; Intel MKL)
  FOSS 2018a (gcc, g++, gfortran; OpenMPI; ScaLAPACK, OpenBLAS, FFTW)
- Note: **Never mix** FOSS and Intel compilers (gives dependency conflict)

Command	Remark
`module av`	List all installed modules
`module av Python`	List all Python-related modules
`module spider Python`	Get more info
`module load Python/3.6.4-intel-2018a`	Load a specific module
`module list`	List all loaded modules and their dependencies
`module unload Python/3.6.4-intel-2018a`	Unload a module (but dependencies still stay)
`module purge`	Remove all modules from your work session

Software: Your Specific Needs

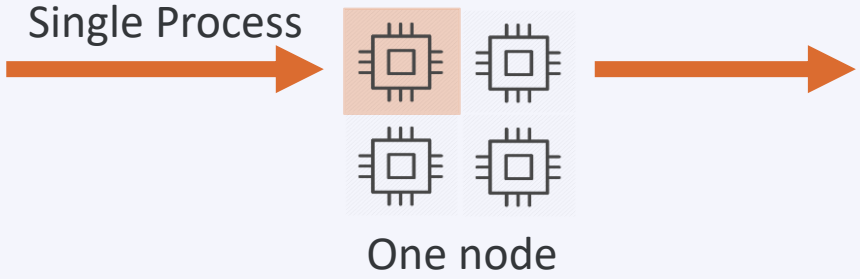
- You can always install your desired software in your $VSC_DATA
  Use Intel or FOSS toolchains
- Compile your code on a compute node (with interactive job)
- If you cannot, ask us for help
- Python/R packages for AI and ML must be installed by the users themselves
- Read more about Python Package Management
- Read more about R Package Management

Starting to Compute

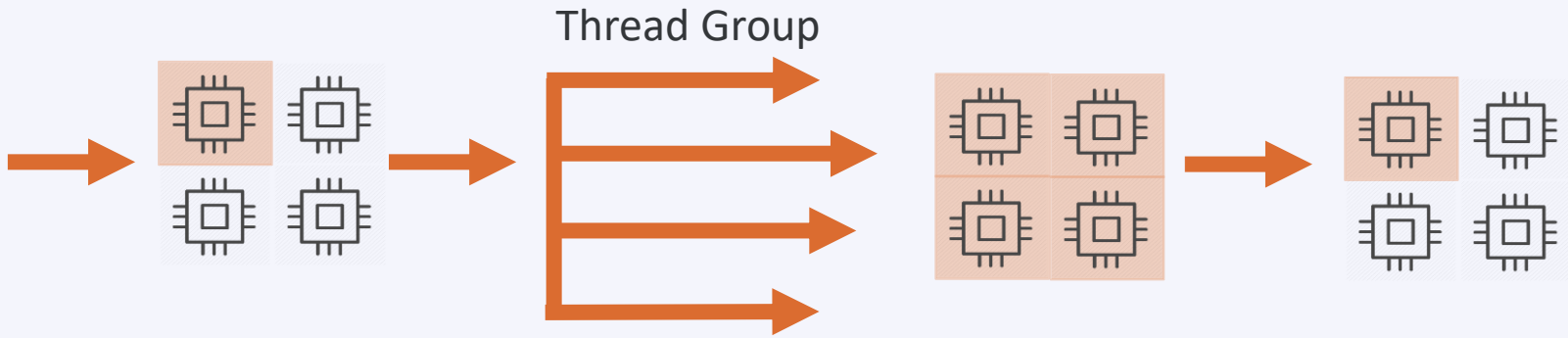
Resource Glossary

- ❑ **Nodes**: how many compute servers to request?
- ❑ **Cores**: how many cores per node to use?
- ❑ **Memory requirement**: how much memory each core needs?
- ❑ **Partition**: gpu, bigmem, superdome, amd
- ❑ **Walltime**: how long to use resources?
- ❑ **Storage**: how much storage (data, scratch, etc) the job needs?
- ❑ **Credits**: how many compute credits will be consumed?

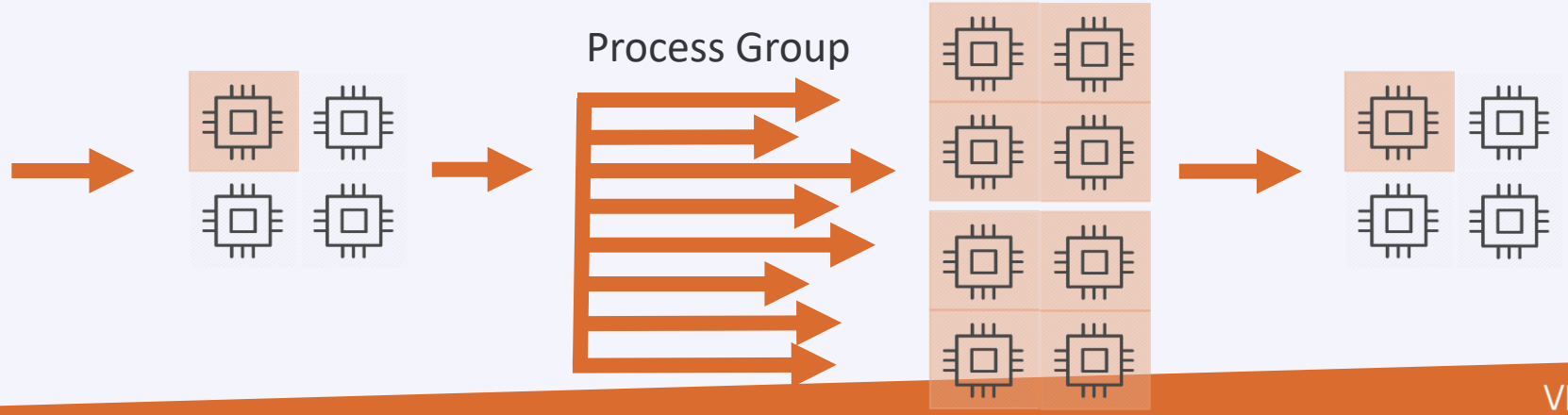
Serial Application
(1 process on 1 core)



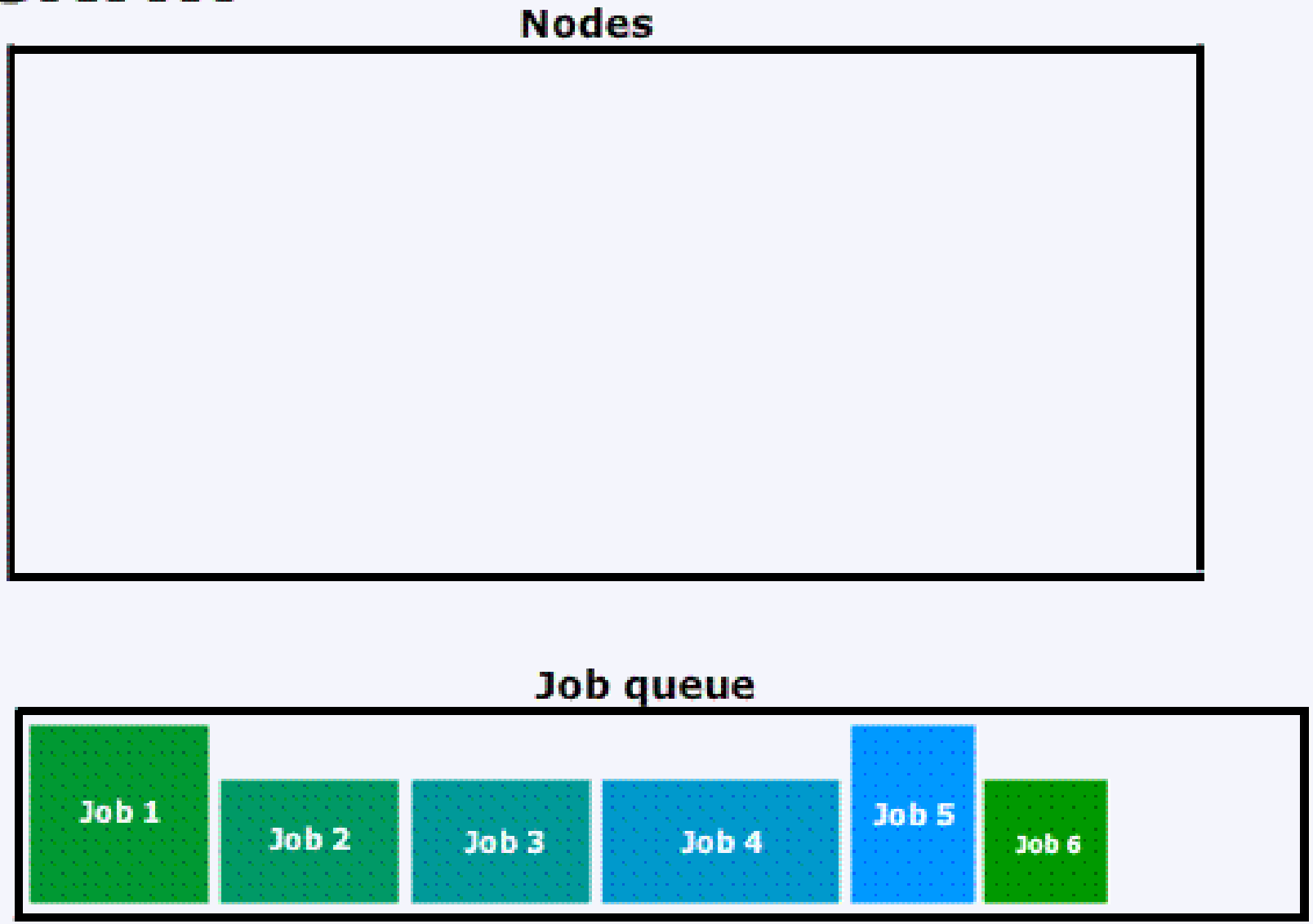
Multi-Core Appl.
(N threads on N cores from 1 node)



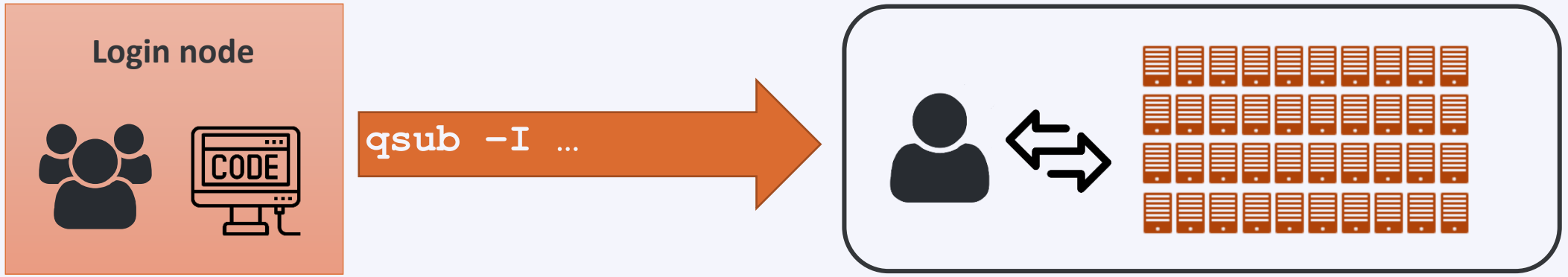
Distributed Appl.
(many processes on many cores/nodes)



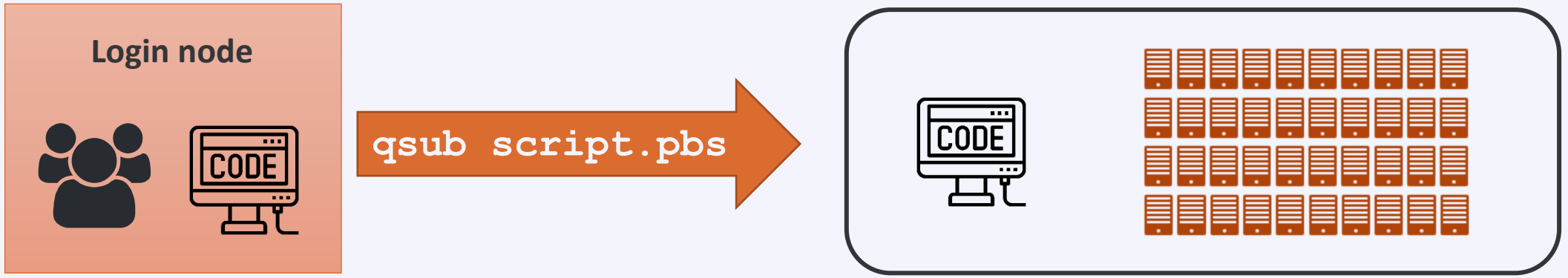
Backfill



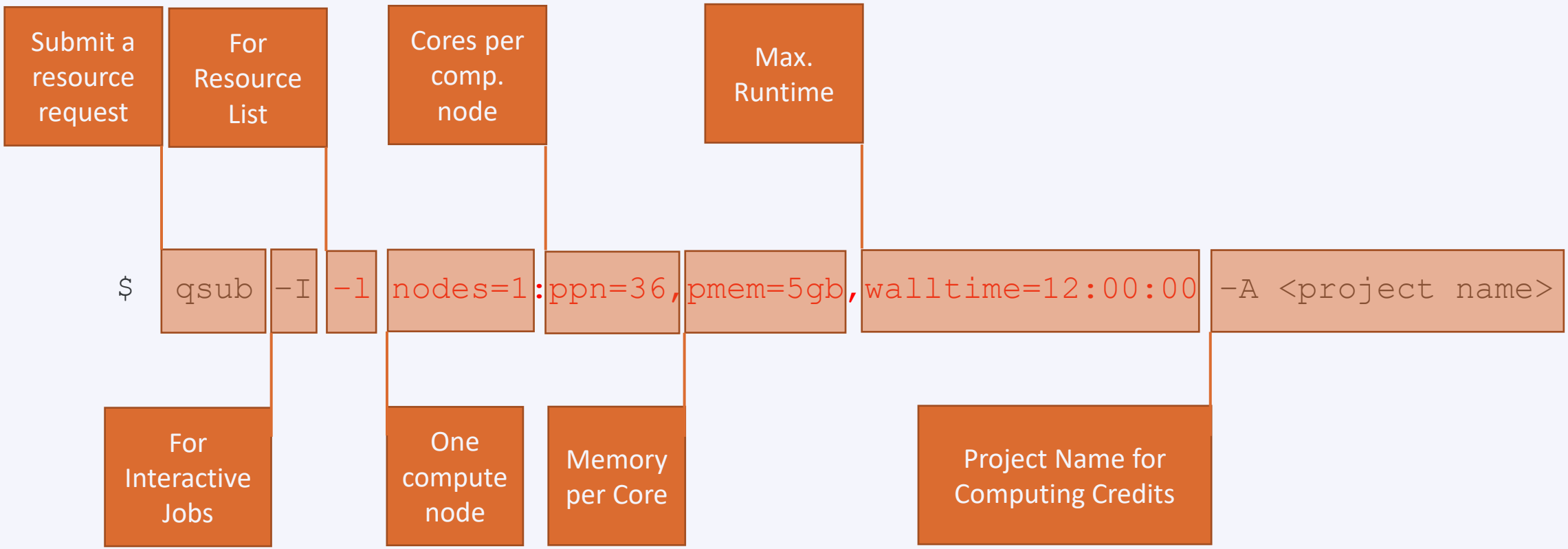
Interactive Job



Batch Job



Requesting Compute Resources Interactively



Remarks

- Specifying <project name> for credits is mandatory, e.g.: **`-A lp_hpcinfo_training`**
- If you request 2000 introductory credits, you use them like: **`-A default_project`**
- Implicit defaults are `nodes=1:ppn=1,pmem=5gb,walltime=1:00:00`

Interactive Jobs

- Interactive job: 1 core for 1 hour (default)

```
$ qsub -I -A lp_hpc
```

- Interactive job with X-forwarding

```
$ qsub -I -X -A lp_hpc
```

- Request fraction of a node

```
$ qsub -I -l nodes=1:ppn=8:cascadelake -A lp_hpc
```

Example: PBS Job Script

```
#!/bin/bash
#PBS -l walltime=00:10:00
#PBS -l nodes=1:ppn=36
#PBS -l pmem=5gb
#PBS -N testjob
#PBS -A lp_hpcinfo_training
#PBS -m ae
#PBS -M my.name@kuleuven.be

module load intel/2018a
which icc

cd $PBS_O_WORKDIR
cp /apps/leuven/training/HPC-intro/cpujob.pbs $VSC_SCRATCH
echo I am done
```

Shebang

Resource List

Module load(s)

Move data

Execure commands

Batch Workload

- Submit the job to the batch server
- Receive a unique JobID
- Error and output files

Job Script

```
#!/bin/bash
…
```

Command Line

```
$ qsub simulation.pbs
```

JobID

```
50041238.tier2-p-
moab2.tier2.hpc.kuleuven.be
```

stderr, stdout

```
$ ls simulation*
simulation.pbs
simulation.pbs.e50041238
simulation.pbs.o50041238
```

Standard Error File

- Always created
- <JobScript>.**e**<JobID>
- Contains all errors and warnings
- If empty: everything went well
- Always study it
- Addess all warnings and errors (if you can)
- Typical error examples …

stderr

```
$ ls *.e*
simulation.pbs.e50041238
```

Job Crash

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

Short Walltime

```
PBS: job killed: walltime 432031 exceeded
limit 432000
```

Low Disk Space

```
IOError: [Errno 122] Disk quota exceeded
```

Standard Output File

- Always created
- <JobScript>.o<JobID>
- Contains all standard output (instead of screen)
- Always study it

stdout

```
$ ls *.o*
simulation.pbs.o50041238
```

Output File

```
time: 3600
nodes: 1
procs: 1
account string: lpt2_sysadmin
queue: q1h
============================
Hello World!
============================
Date: Fri Mar 20 14:32:01 CET 2020
Allocated nodes:
r26i27n11
Job ID: 50240161.tier2-p-moab-2.tier2.hpc. …
Resource List:
pmem=5gb,walltime=01:00:00,neednodes=1:ppn=36
Resources Used:
cput=00:00:01,vmem=0kb,walltime=00:00:04,mem=0kb,e
nergy_used=0
Queue Name: q1h
----------------------------
time: 4
nodes: 1
procs: 1
account: lpt2_sysadmin
```

Summary

stdout

Resources

summary

Other Partitions

GPU

```
#PBS -l partition=gpu
#PBS -l
nodes=1:cores=9:gpus=1:skylake
#PBS -l pmem=5gb
```

Big Memory

```
#PBS -l partition=bigmem
#PBS -l nodes=1:cores=36
#PBS -l pmem=20gb
```

AMD

```
#PBS -l partition=amd
#PBS -l nodes=1:cores=64
#PBS -l pmem=3800mb
```

Superdome

See VSC documentation

Managing & Monitoring Jobs

Command	Purpose
`$ qsub ….`	Submit a job (batch/interactive)
`$ qdel <JobID>`	Delete a specific job
`$ mycheckjob <JobID>`	Diagnose issues with your job, if any
`$ 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`
`$ clusterview`
`$ queueview`
	Overview of the cluster
	Overview of the nodes, cores and GPUs
	Overview of the job queues

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

Debugging / Testing Jobs

- To quickly test/debug your (parallel) application
- 2 dedicated nodes on ThinKing and Genius
  One GPU node and one CPU node
- 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=1:ppn=10 -l qos=debugging -l \
       walltime=30:00 -A default_project
```

Singularity Containers

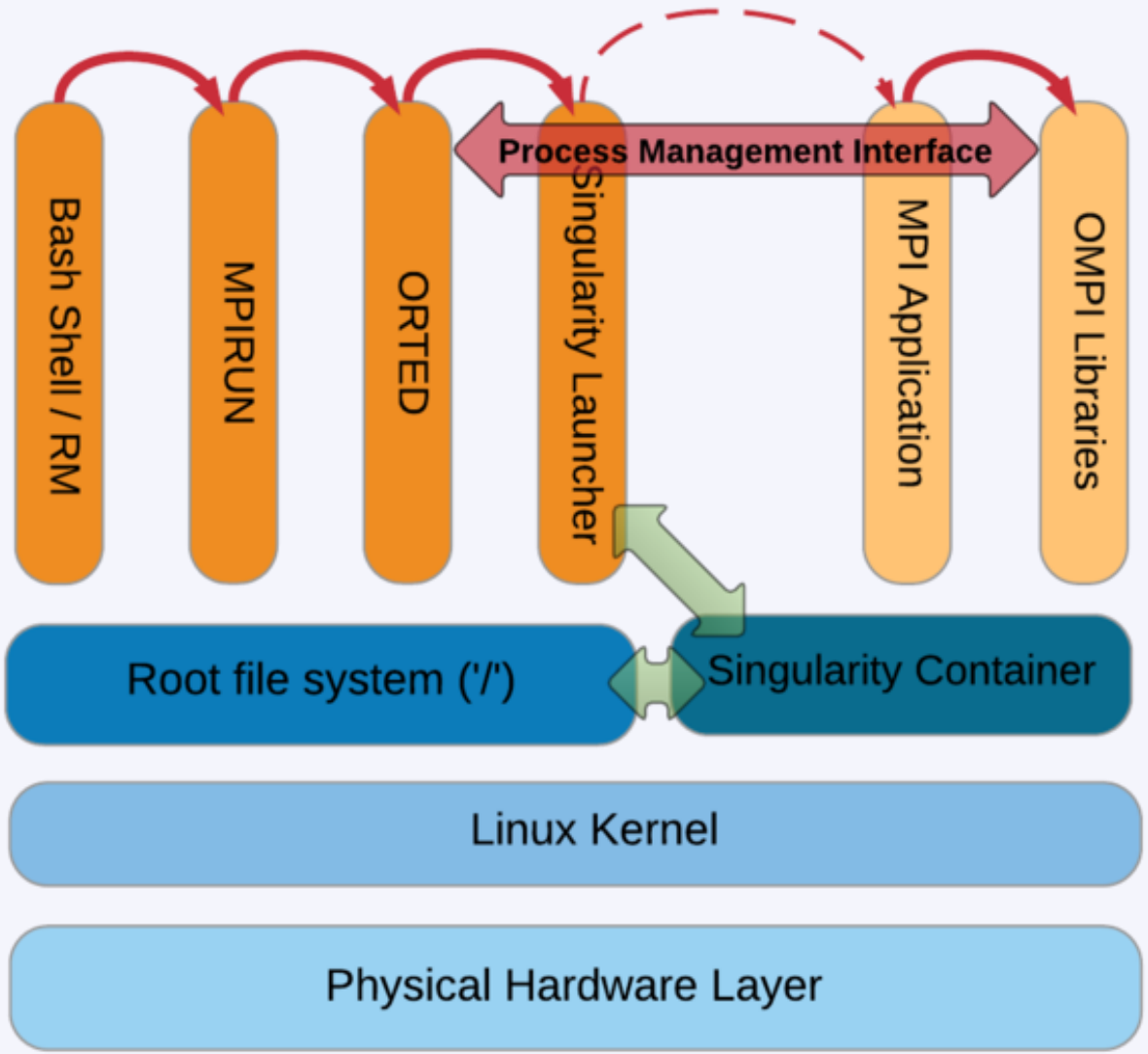
- What?
  + Self-contained OS & software & data
- Why?
  + fully resolved dependency chains
  + portable workflow
- How?
  + You create the image
  + Run it on Genius
  + MPI/OpenMP is supported

PBS Script

```
#!/bin/bash -l
#PBS -l walltime=00:30:00
#PBS -l nodes=4:ppn=36:pmem=5gb
#PBS -A lp_hpcinfo_training

cd $PBS_O_WORKDIR

singularity run Project.simg ./model.exe
```



Credit Pricing

- You pay as you go!
- For academic projects:
  1000 credits = 3.5 EUR
- Credits needed for a job:

  #credits = Walltime (hr) × #nodes × Factor

- For shared nodes, you pay a fraction of the costs, based on the ppn specified

Cluster / Partition	Credits/hr
Genius Cascadelake	11.3
Genius Cascadelake 8 GPUs	40
Genius Skylake 4 GPUs	20
Genius Skylake BigMem	12
Genius Skylake	10
Genius / Superdome	10
Genius / AMD nodes	10
ThinKing / Haswell	6.68
ThinKing / IvyBridge	4.76

How to Manage Credits?

Command	Purpose
`mam-balance`	List active projects and available credits
`mam-list-allocations`	List the validity dates of different projects/allocations
`mam-list-chargerates`	List current charge rates for different nodes
`mam-list-accounts -a <account-name>`	List the members in an account

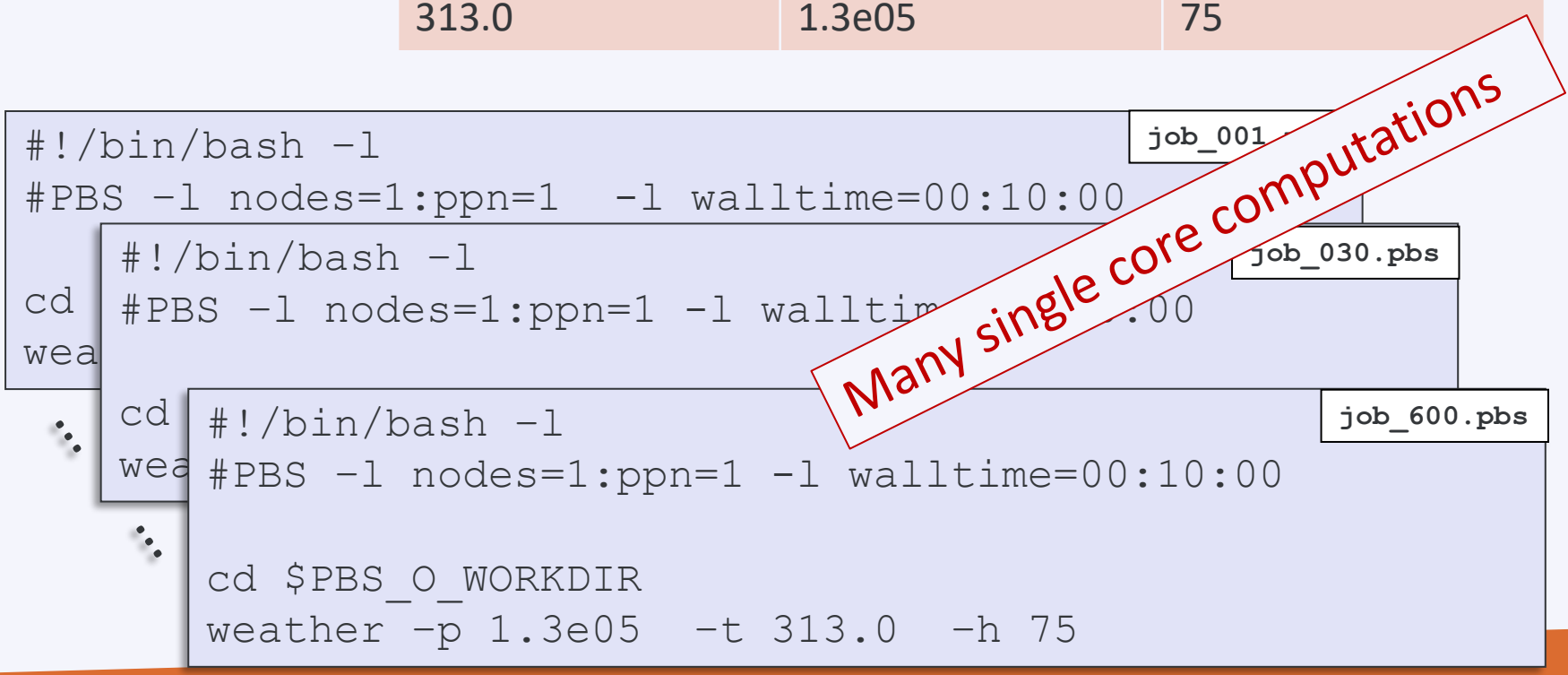
Worker Framework

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

Use case: parameter exploration

temperature	pressure	humidity
293.0	1.0e05	87
…	…	…
313.0	1.3e05	75



Solution: worker with -data

temperature	pressure	humidity
293.0	1.0e05	87
…	…	…
313.0	1.3e05	75

data.csv

job.pbs

```
#!/bin/bash -l
#PBS -l nodes=5:ppn=20  -l walltime=01:20:00

cd $PBS_O_WORKDIR
weather -p $pressure  -t $temperature  -h $humidity
```

```
$ module load worker
$ wsub  -data data.csv  -batch job.pbs
```

Data exploration: steps

- Write PBS script with parameters
- Create Excel sheet with data
  - Convert to CSV format
- Submit with `wsub`
  - walltime is time to complete all work items

$$walltime_{\text{job}} \geq \frac{N \cdot walltime_{\text{work item}}}{nodes \cdot ppn}$$

Demo: Test for yourself

demo/test yourself

- Request membership to lp_hpcintro_training group (account.vscentrum.be)

- Login with putty
- Filetransfer with Filezilla
- Login with NX
- Check disk quota
- Check the credits
- Check/load/list/unload/purge module

demo/test yourself

- Copy intro training files (`/apps/leuven/training/HPC_intro/`) to your `$VSC_HOME`
- Submit `cpujob` to the cluster
- List all your jobs (`qstat`)
- Check the information about the cpujob (`checkjob`)
- Modify the mat.pbs script to request 1 node, 36 cores for 30 minutes and get the notification about job start/end by e-mail
- Check the status of all the jobs

demo - monitoring

- Submit an interactive job
  Run your program on a compute node
  Open a new terminal and ssh to a compute node
  Check the resources usage (`top, htop`)

demo – conda usage

- Create a conda environment including Jupyter

```
$ conda create -n science jupyter numpy scipy
```

- Activate this environment

```
$ source activate science
```

- Add matplotlib package to this environment

```
$ conda install matplotlib
```

- Return to original environment

```
$ conda deactivate
```

demo – notebooks

- Start an interactive GPU job

```
$ qsub -I -l walltime=30:00 -l nodes=1:ppn=9:gpus=1 -l partition=gpu -A default_project
```

- Activate conda environment

```
$ source activate science
```

- Go to your working directory (you can use `$PBS_O_WORKDIR` if you qsub from there)
  Start notebook

```
$ jupyter notebook --port ${USER:3} --ip $(hostname)
$ jupyter notebook --port 30468 --ip $(hostname)
```

- Open the link in the browser in NX and test your notebook

demo – worker

- Copy intro training files (`/apps/leuven/training/worker/`) to your `$VSC_HOME`
- Go to `exercise1` directory
- Submit worker job
- Check the output file

Questions

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

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