HPC@UAntwerp introduction

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Version Fall 2025 – Part 1

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1 — Introduction to the VSC

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CalcUA and VSC

- **HPC core facility CalcUA**
  - provides HPC infrastructure & software for researchers
  - offer training & support
  - UAntwerp Tier-2 infrastructure (local)

- **Vlaams Supercomputer Centrum** (VSC)
  - partnership between 5 University associations: Antwerp, Brussels, Ghent, Hasselt, Leuven
  - FWO funded (Research Fund – Flanders)
  - goal: make HPC available to all researchers in Flanders – academic and industrial
  - provides central **Tier-1** infrastructure
  - other local **Tier-2** infrastructures: VUB, UGent and KU Leuven / UHasselt

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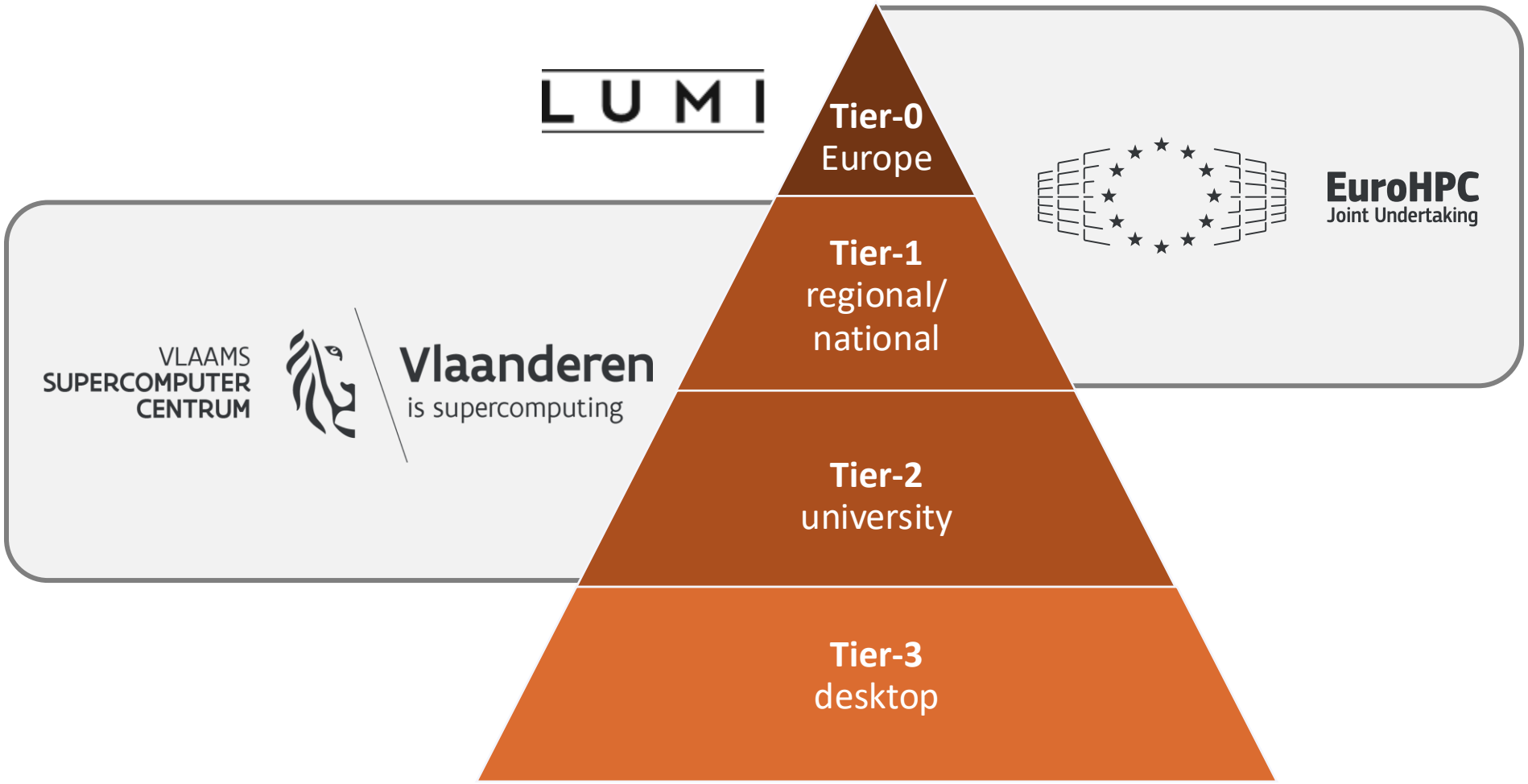
The European HPC landscape



UAntwerp Tier-2 infrastructure

UAntwerp Tier-2 Infrastructure

Leibniz

2 login nodes

152 compute nodes
- Intel Broadwell
- 2x 14 cores

2 GPU nodes
- 2x Nvidia P100

vector engine node

visualisation node

Vaughan

2 login nodes

152 compute nodes
- AMD Rome (Zen 2)
- 2x 32 cores

40 compute nodes
- AMD Milan (Zen 3)
- 2x 32 cores

1 GPU node
- 4x Nvidia A100

2 GPU nodes
- 2x AMD MI100

storage system
shared, 730 TB

Breniac

Login node

23 compute nodes
- Intel Skylake
- 2x 14 cores

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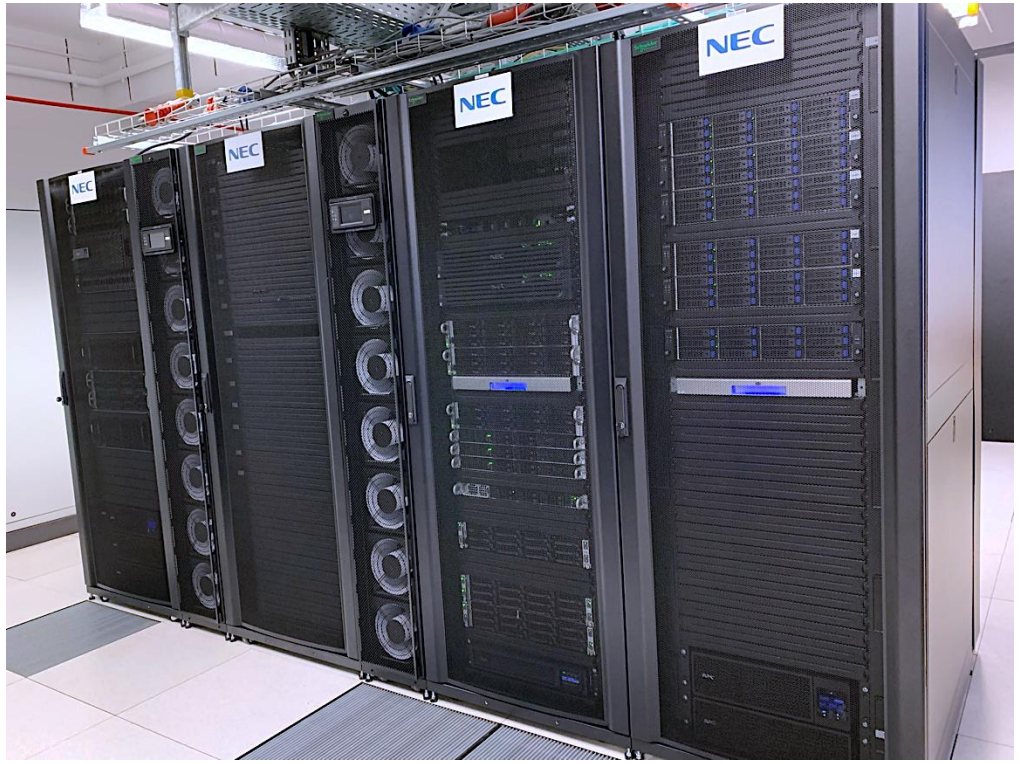
UAntwerp Tier-2 infrastructure



CalcUA VSC

\Orchestrating a brighter world

NEC

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VSC Tier-1 infrastructure

VSC Tier-1 Infrastructure

Hortense (UGent)

2 Login nodes

384 compute nodes
- AMD Rome (Zen 2)
- 2x 64 cores

20 GPU nodes
- 4x Nvidia A100

PHASE 2

384 compute nodes
- AMD Milan (Zen 3)
- 2x 64 cores

20 GPU nodes
- 4x Nvidia A100

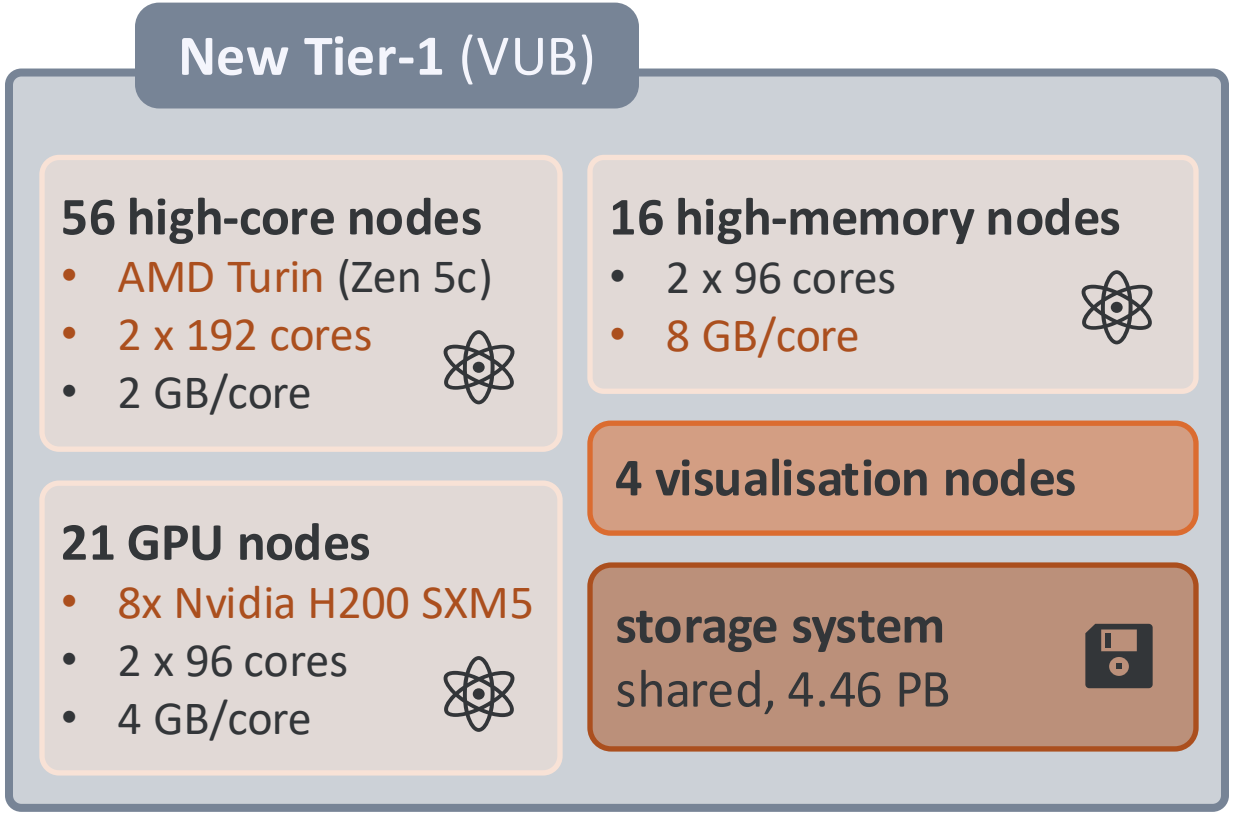
Storage system
shared, 5.4 PB

VSC Tier-1 infrastructure

Hortense (UGent)

New VSC Tier-1 infrastructure — Operational in 2026

- Flanders invests €8.6 million in the purchase of a new Flemish supercomputer
  - VUB to host and manage the supercomputer at Research Park Zellik



Characteristics of a HPC cluster

- **Shared infrastructure**, used by multiple users simultaneously
  - you need to request the appropriate resources
  - you may have to wait a while before your computation starts
- Expensive infrastructure
  - **software efficiency matters!**
- Built for parallel jobs
  - **no parallelism = no supercomputing**
  - not meant for running a single one-core job
- Remote computation model
  - for *batch computations* rather than interactive applications
- Linux-based systems
  - no Windows or macOS software

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2 — Connect to the cluster

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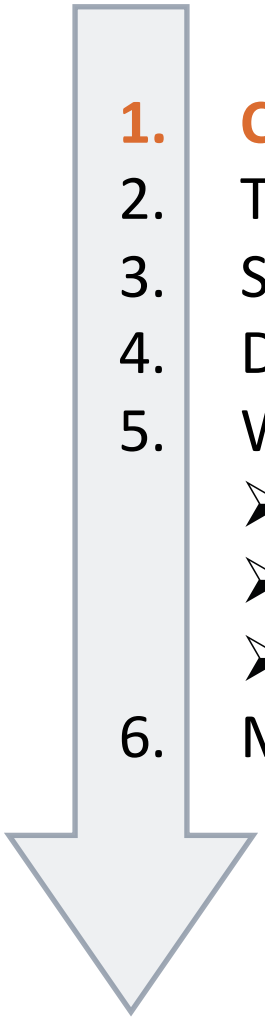
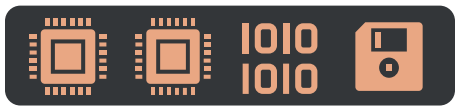
A typical workflow



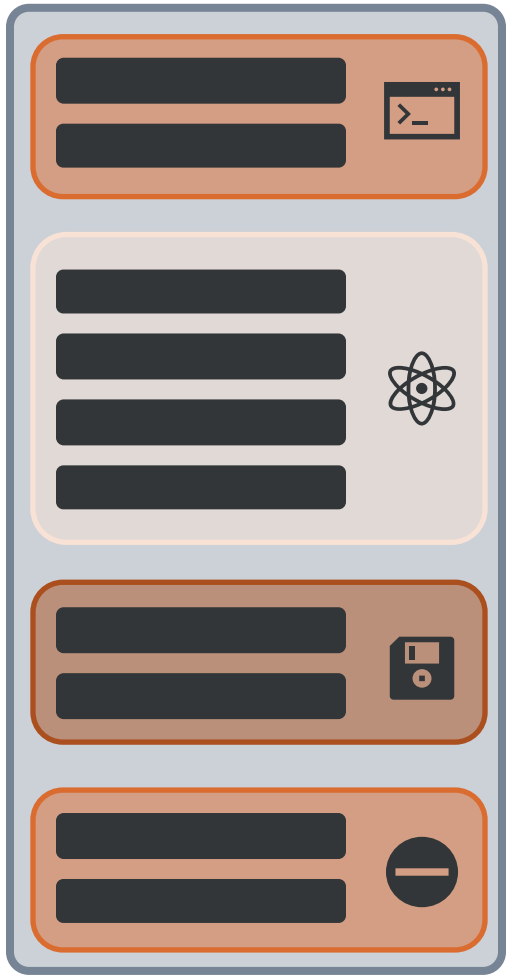
1. **Connect to the cluster**
2. Transfer your files to the cluster
3. Select the software and build your environment
4. Define and submit your job
5. Wait while
   - ➢ your job gets scheduled
   - ➢ your job gets executed
   - ➢ your job finishes
6. Move your results

Types of cluster nodes

- Computer cluster consists of nodes
  - each node has specific task(s)



- Login nodes
  - SSH access to the clusters
  - edit & submit jobs
  - small compilations
- **New: Open OnDemand web portal**
  - web access to the clusters
- Compute nodes
  - actual computations



Login section

Compute section

Storage section

Admin section

Web portal access — New

Open OnDemand web portal

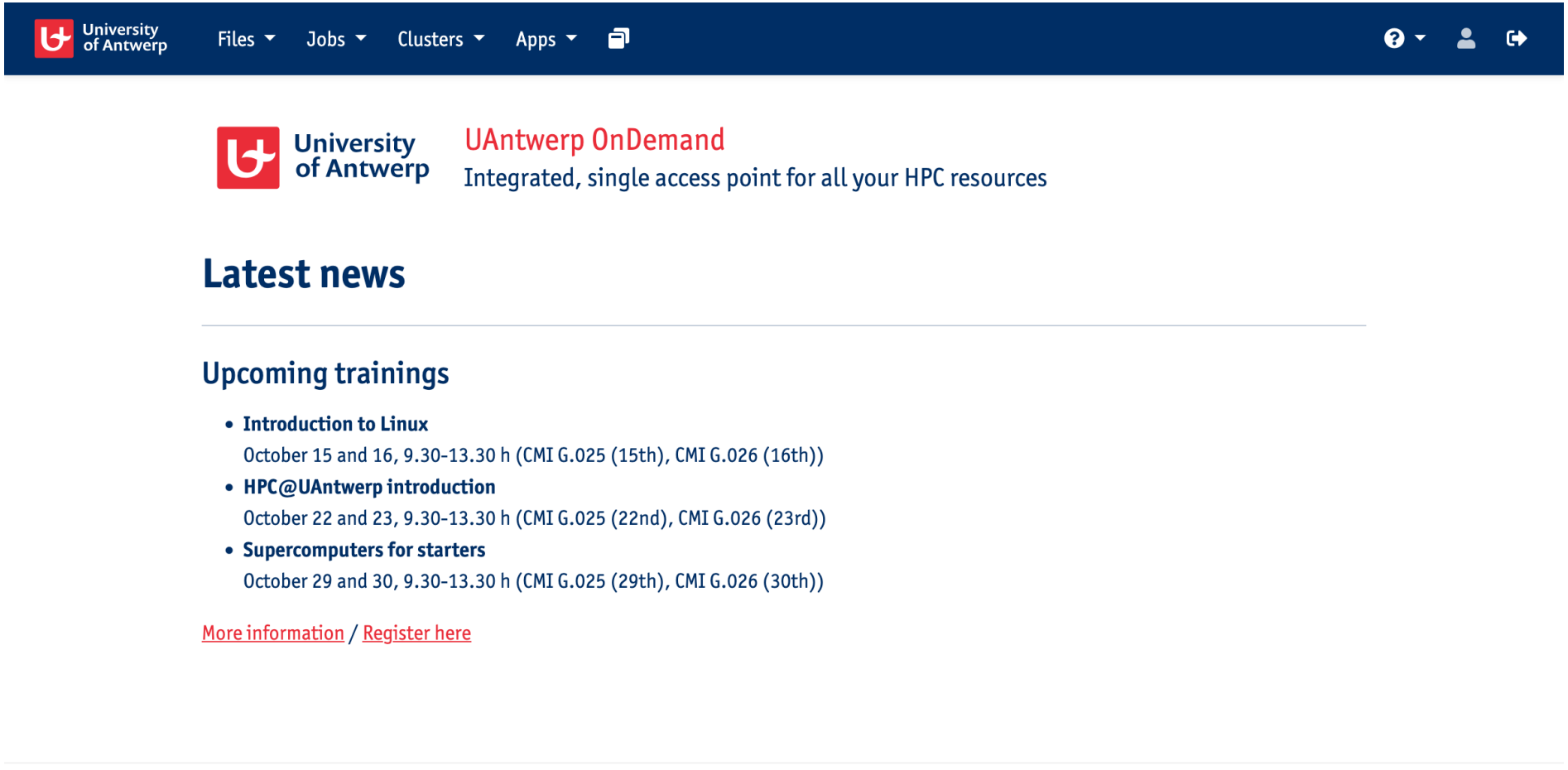
- Provides a user interface to HPC clusters from within a web browser
  - browse, create, transfer, view and/or edit files
  - open a shell on one of the login nodes
  - submit and monitor your jobs
  - create job templates

- Use interactive applications
  - interactive shell on the compute nodes, or desktop sessions
  - programming environments — e.g., VS Code, JupyterLab, RStudio

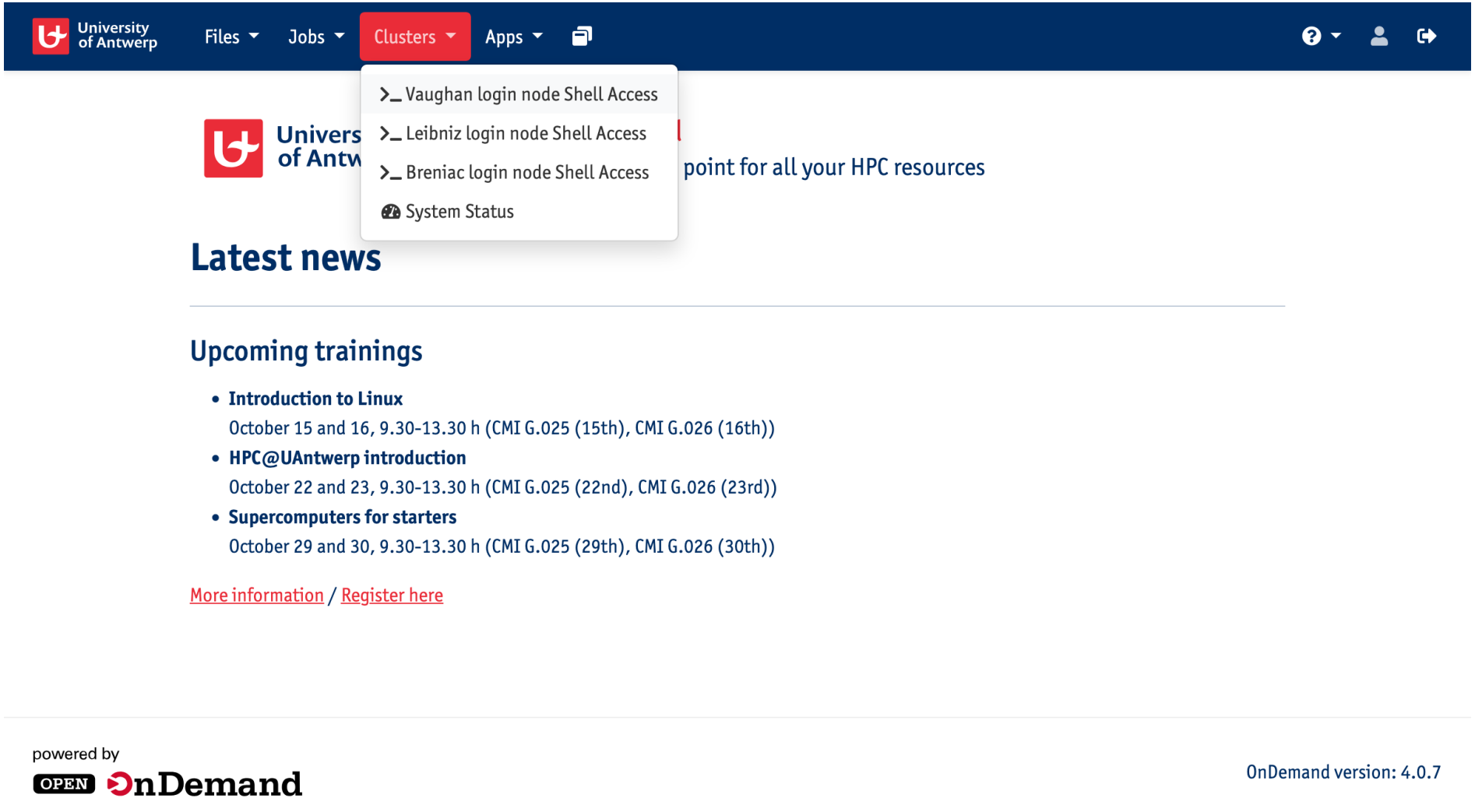
- Log in with UAntwerp or VSC account — *no SSH keys required!*

Open OnDemand

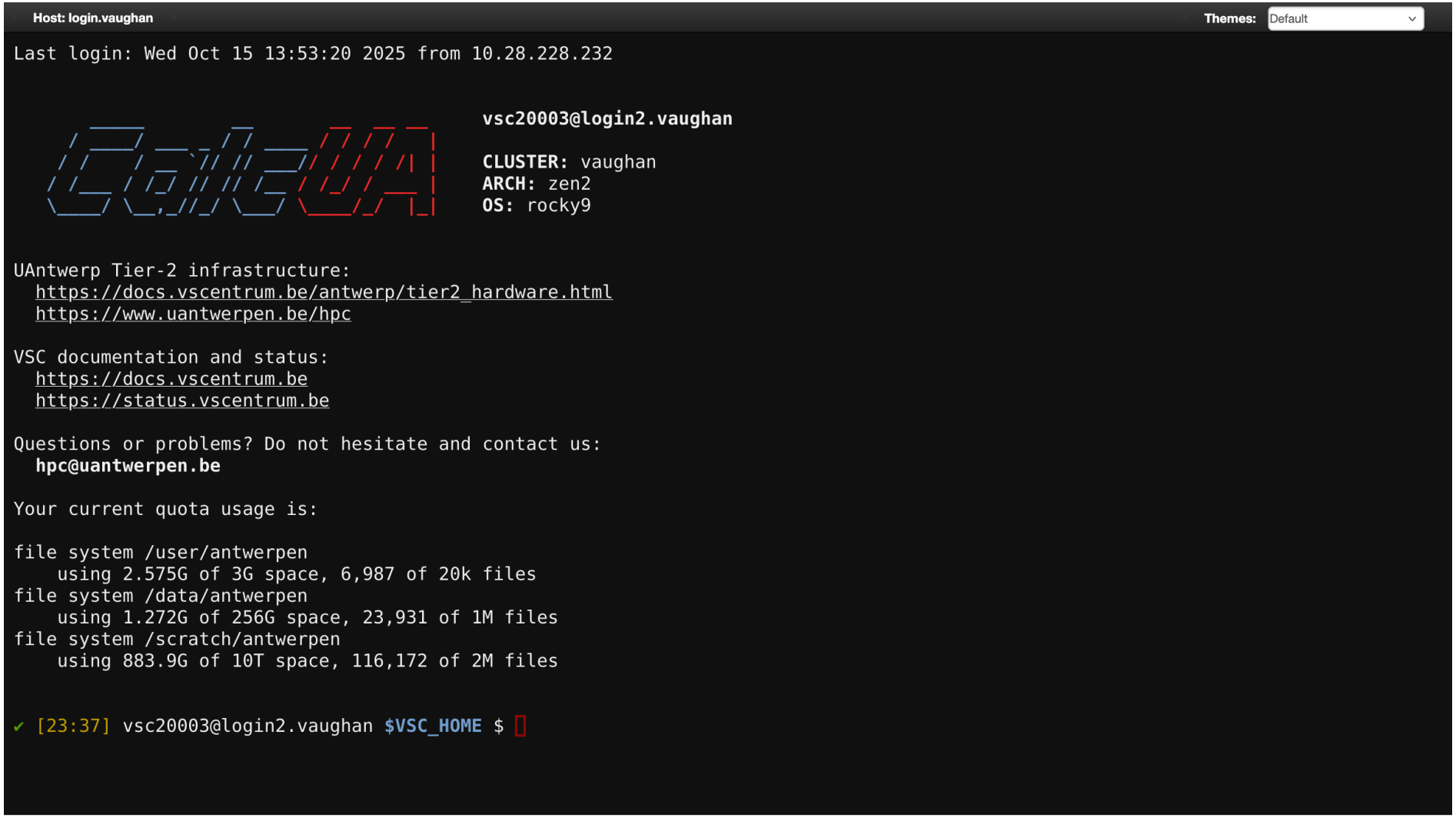
Web portal access — https://portal.hpc.uantwerpen.be



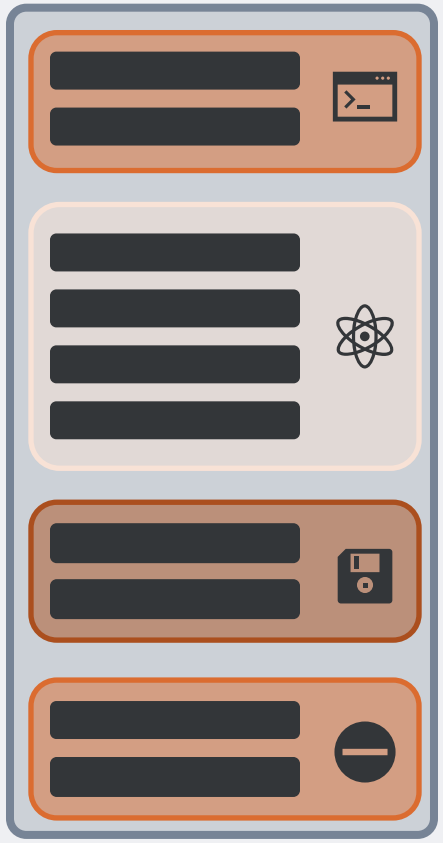
Web portal access — Connect to the cluster



Web portal access — Connect to the cluster



Summary — Access to a HPC cluster



- A HPC cluster is **shared infrastructure** with multiple users
- It consists of many nodes with different functions: login nodes, compute nodes, storage nodes, …
- You access the machine through the **login nodes**
  - web portal: *login node shell access*
- You **request** a **compute** allocation for your computations
  - **batch scripts** (see 5 - define and submit your job)
  - web portal: *interactive shell*

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3 — Transfer your files to the cluster

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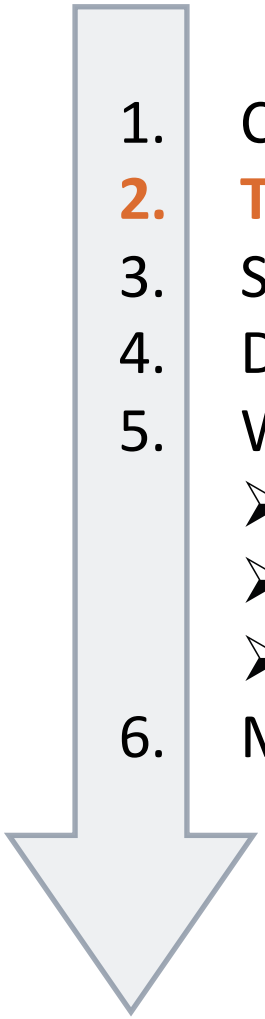
A typical workflow



1. Connect to the cluster
2. **Transfer your files to the cluster**
3. Select the software and build your environment
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5. Wait while
   - ➢ your job gets scheduled
   - ➢ your job gets executed
   - ➢ your job finishes
6. Move your results

File systems and user directories

- `/scratch/antwerpen/2xx/vsc2xxyy`
  - fast but temporary storage
  - highest performance – for large files
  - local only, no backup

`$VSC_SCRATCH`

- `/data/antwerpen/2xx/vsc2xxyy`
  - long-term storage
  - slower – for small files
  - exported to other VSC sites

`$VSC_DATA`

- `/user/antwerpen/2xx/vsc2xxyy`
  - only for account configuration files
  - exported to other VSC sites

`$VSC_HOME`

Block and file quota limits

- Block quota limits the *size of data*
- File quota limits the *number of files*

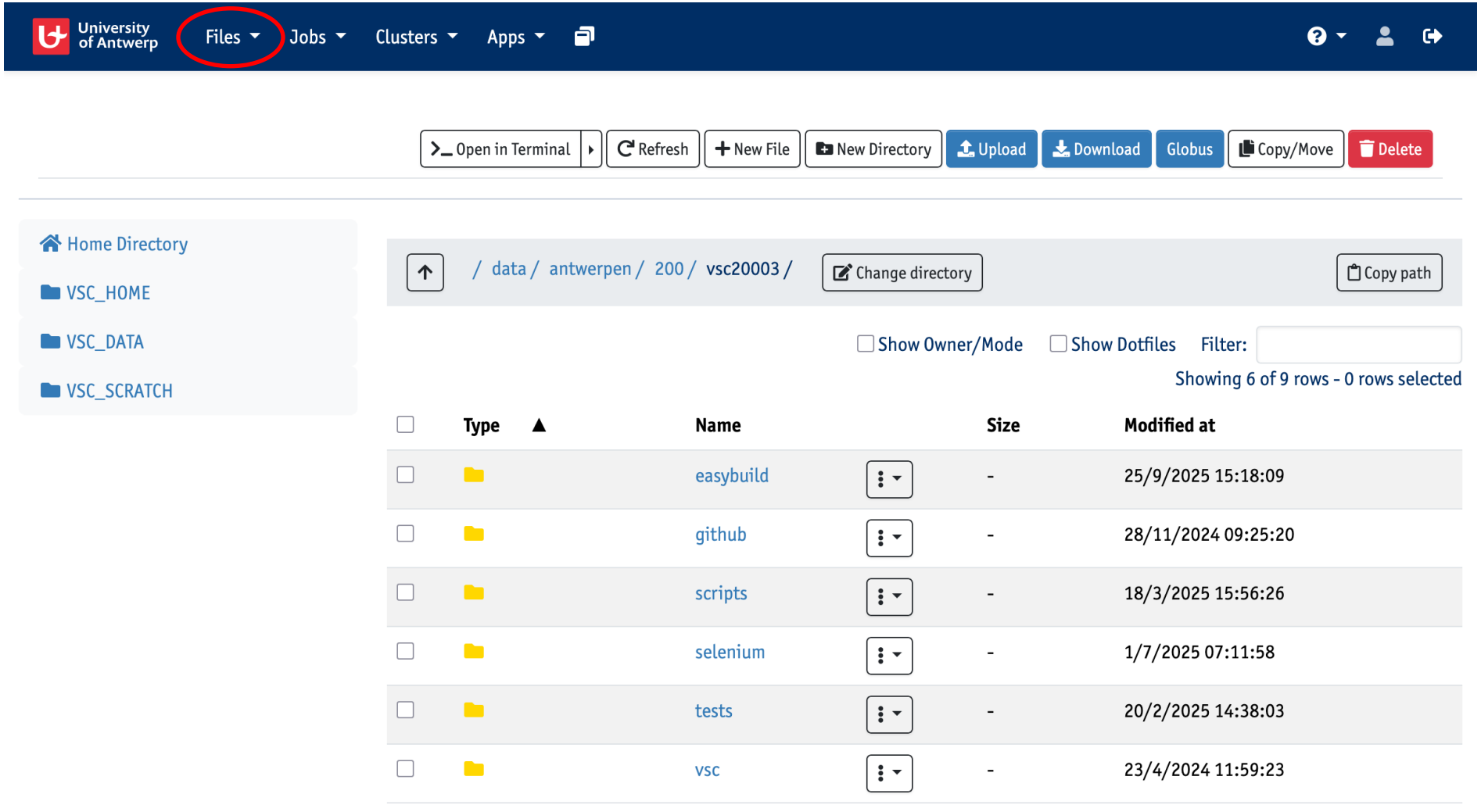
- Default values (but you can request more)

File system	Block quota	File quota
/scratch	50 GB	100 k
/data	25 GB	100 k
/home	3 GB	20 k

  - Show quota: at login or with the `myquota` command

- Note: on /scratch, the number of files corresponds to number of data *chunk* files
  - 1 end-user created file can be spread over at most 8 data chunk files
  - does not include the number of directories

Web portal access — Transfer your files



Globus — Data sharing platform

Globus web interface

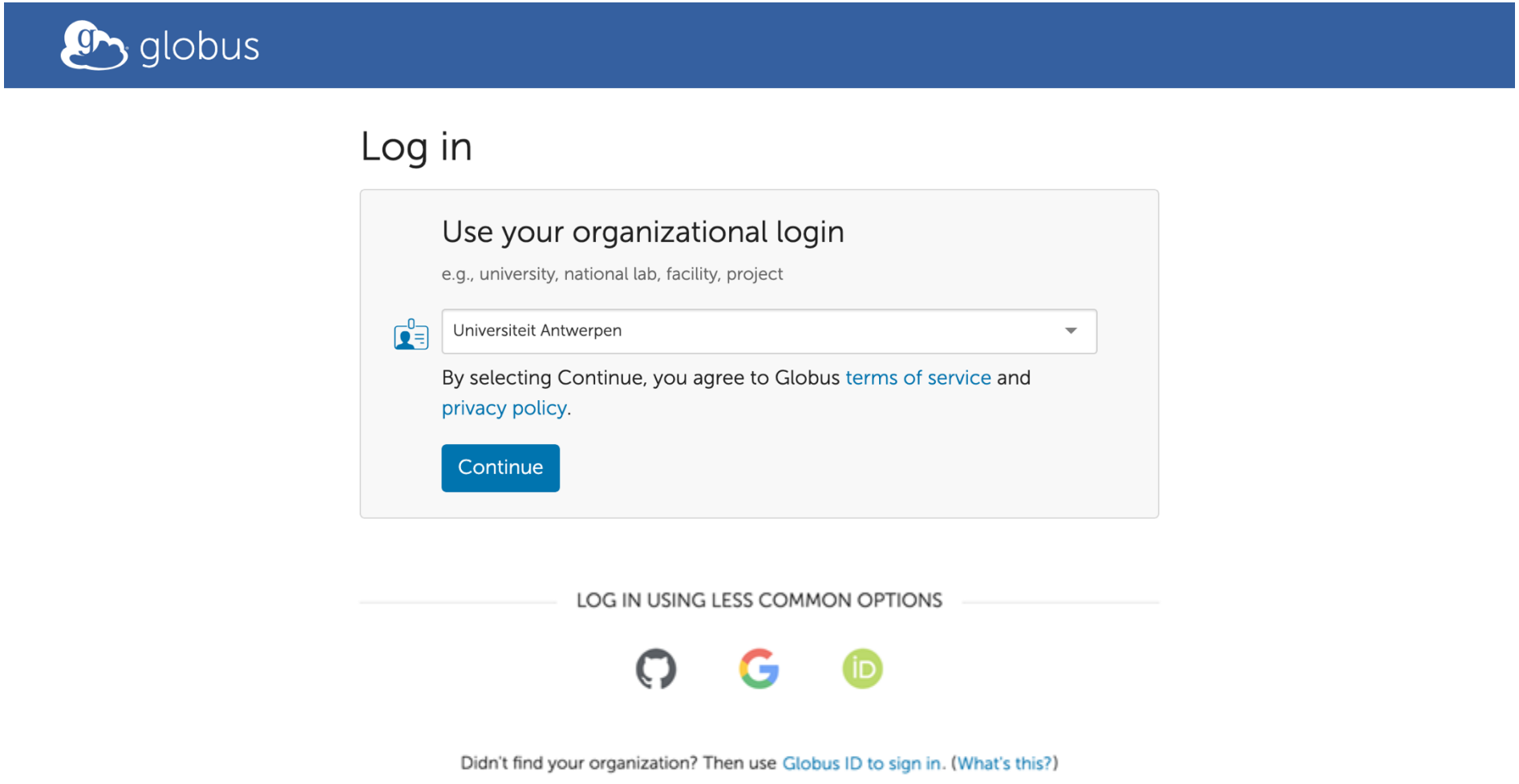
- Web app to transfer large amounts of data between local computer and/or remote servers
  - offers premium data sharing features, guest collections and connectors (e.g., for OneDrive)
  - transfers will resume automatically, synchronization options available
  - has a command-line interface as well as a Python SDK

- HPC@UAntwerp collection: **VSC UAntwerpen Tier2 filesystems**
  - access to both user and shared group directories
  - log in with UAntwerp or VSC account — *note: active VSC account needed*

- Transfer from/to local computer (laptop/desktop): Globus Connect Personal
- Transfer between remote servers*: no local software needed!*

Globus data sharing platform — Overviews & Concepts

Globus — Data sharing platform



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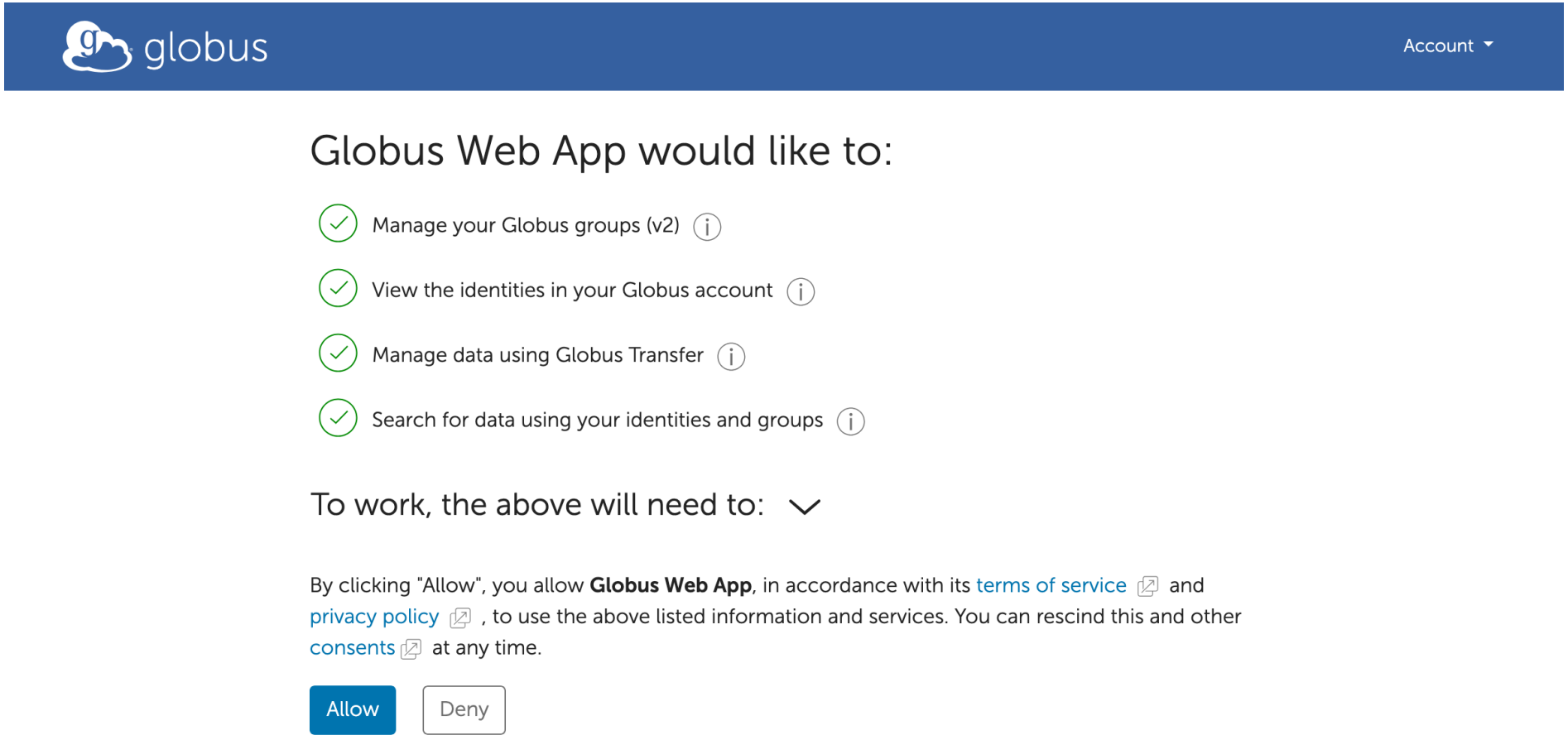

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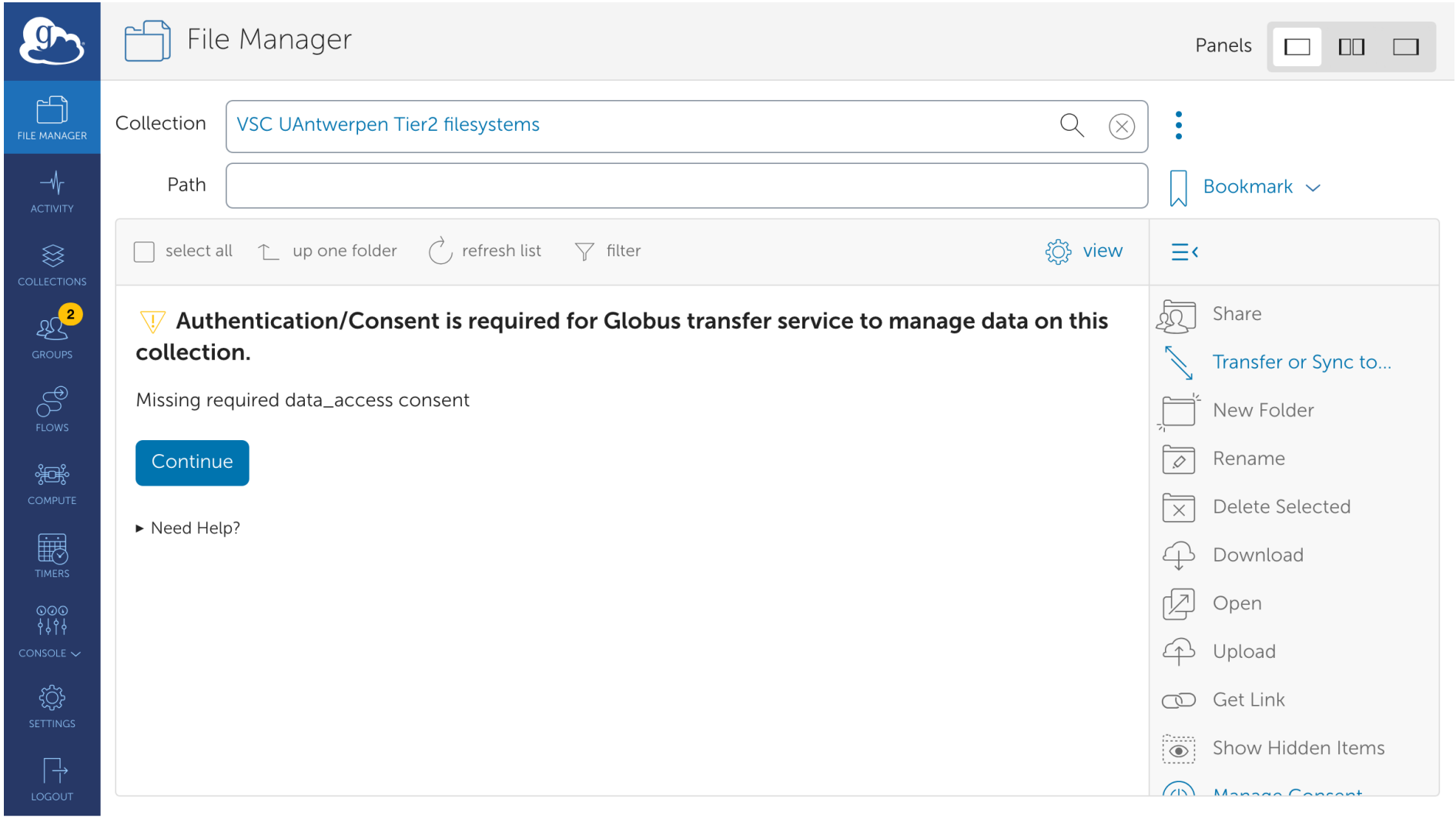
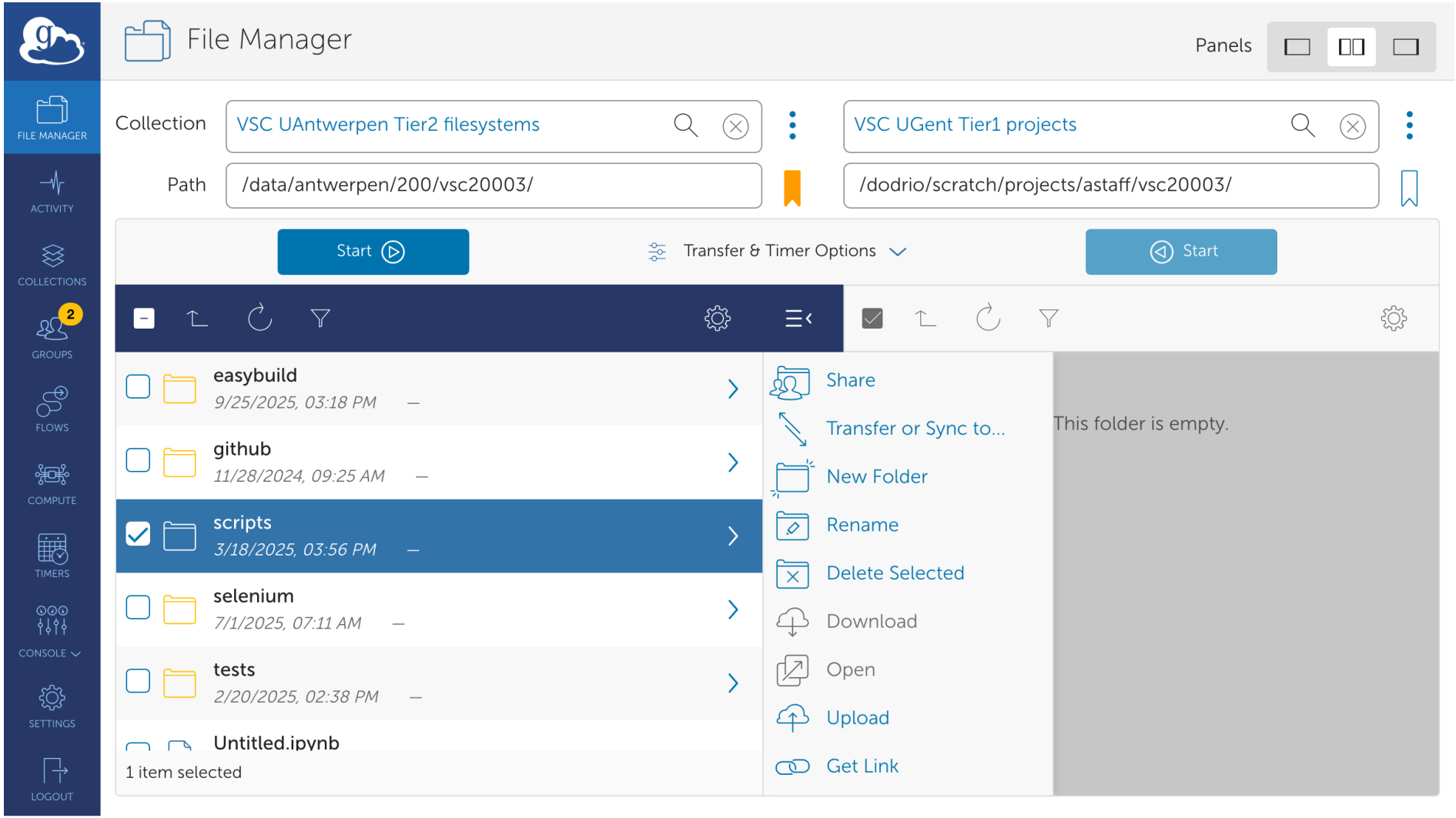


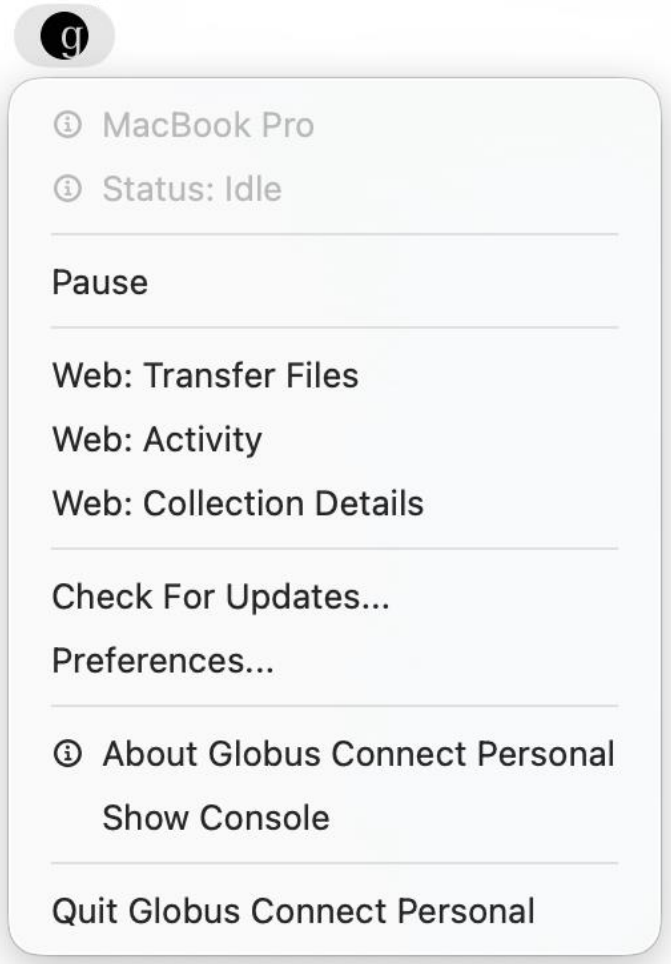
Globus — Transfer between remote servers



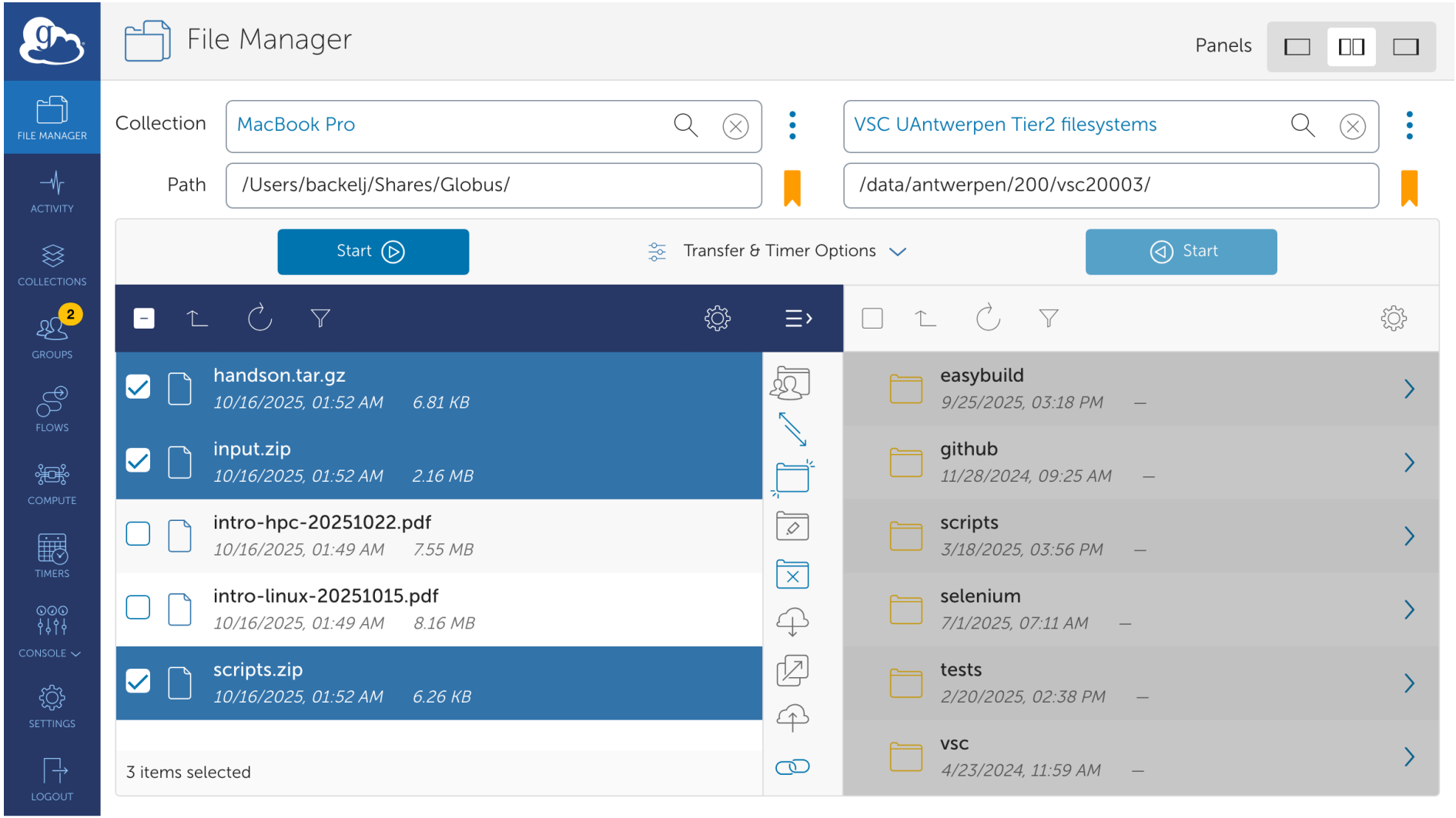
Globus — Transfer from/to local computer

Globus Connect Personal

- Create a local collection for your laptop/desktop
  - easily and reliably move and share large amounts of data
  - easily synchronize folders repeatedly — e.g., for back up
  - interact with other Globus collections — e.g., VSC …
  - transfers will resume automatically
- *Warning: be careful when setting accessible directories*
  - e.g., only allow access to dedicated directory for Globus
  - by default, your home directory is selected, so *remove it*



Globus — Transfer from/to local computer



Best practices for file storage

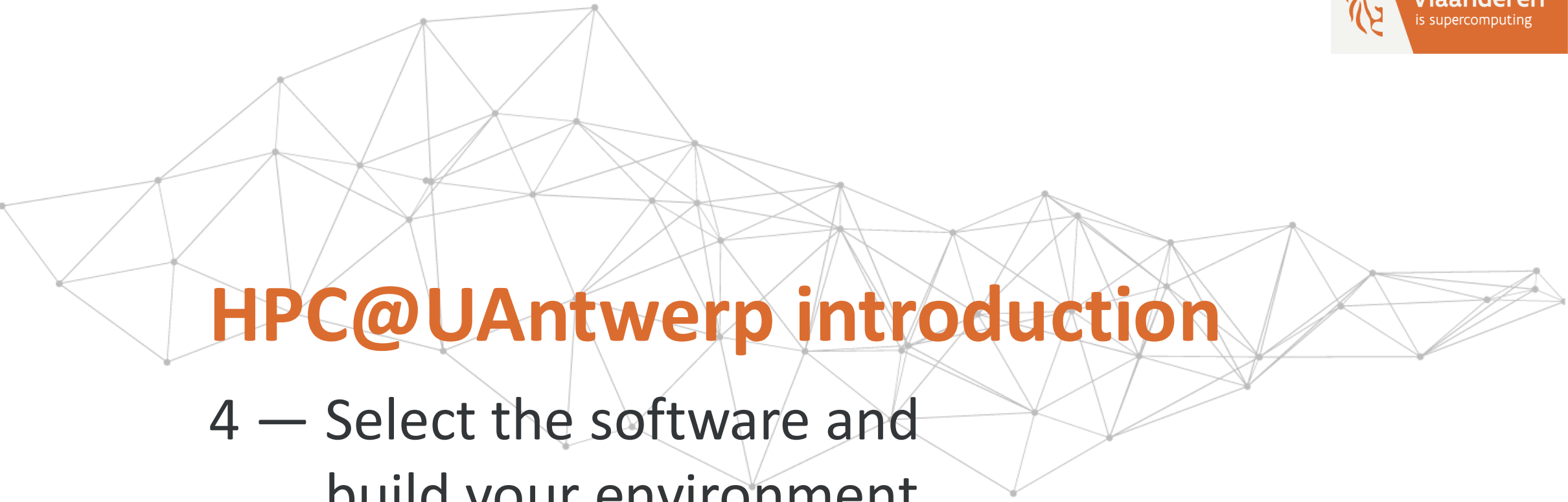
- **The cluster is not for long-term file storage**
  - move back your results to your laptop or server in your department
  - backup exists for `/user` and `/data` – not for very volatile data
  - old data on `/scratch` can be deleted if scratch fills up
- Cluster is optimised for parallel access to large files
  - not for tons of small files (e.g., one per MPI process)
- Request more quota on `/scratch`
  - block quota – without too much motivation
  - file quota – you will have to motivate why you need more files
- *Note: text files are good for summary output, or data for a spreadsheet, but not for storing 1000x1000-matrices — use binary files for that!*

Hands-on

- Copy some files between your laptop and CalcUA
  - using the webportal as well as using the Globus web app
  - copy them back to your laptop with both tools
  - transfer a directory as well
- Download and install Globus Connect Personal
  - login with vsc2xxxx@vscentrum.be
  - choose a name for your collection — e.g. `<name>-laptop`
  - good practice: configure it to use a dedicated subdirectory only — e.g. `~/Globus`
  - initiate a transfer from CalcUA to your laptop
    - look at the options

Summary — Transfer your files to the cluster

- There are 3 user directories:
  - `$VSC_SCRATCH` - data you need for calculations (large files)
  - `$VSC_DATA` - software or data you regularly need on multiple VSC sites
  - `$VSC_HOME` - config files only
- Regularly **back up** your files
  - transfer them using **Globus** or `scp`/`sftp`



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4 — Select the software and build your environment

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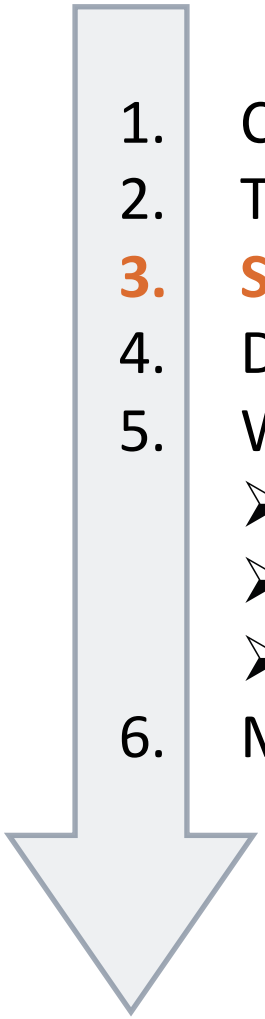
A typical workflow



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System software

- Operating system: **Rocky Linux** – currently, version 9.6
  - Red Hat Enterprise Linux (RHEL) clone
  - Installed on all CalcUA clusters: Vaughan, Leibniz and Breniac
    - All clusters are kept in sync as much as possible
- Resource management and job scheduler: **Slurm**
- Software build and installation framework: **EasyBuild**
- Environment modules system: **Lmod**

Development software

- C/C++/Fortran compilers
  - Intel oneAPI, AOCC, GCC
  - with OpenMP support
- Message passing libraries
  - Intel MPI, Open MPI
- Mathematical libraries
  - Intel MKL, OpenBLAS, FFTW, MUMPS, GSL, …
- File formats and data partitioning
  - HDF5, NetCDF, Metis, …
- Scripting and programming languages
  - Python, Perl, R, …

Application software

- Quantum Chemistry / Computational Chemistry / Electronic Structure Calculations
  - ABINIT, CP2K, QuantumESPRESSO, *VASP*, *Gaussian*, *ORCA*, NWChem, OpenMX, Siesta
- Molecular Dynamics (MD) and Biomolecular Simulation
  - GROMACS, NAMD, AMBER, LAMMPS, CHARMM, Desmond, Tinker, DL_POLY
- Computational Fluid Dynamics (CFD) – TELEMAC, OpenFOAM
- Optimization and Operations Research – Gurobi, CPLEX
- Bioinformatics / Computational Biology – BLAST, Bowtie, Guppy, MAFFT, HMMER, Nextflow
- Data Analysis / Statistical Computing / Scientific Computing – *MATLAB*, R, Python (SciPy/NumPy), Julia
- Machine Learning / AI / Deep Learning Frameworks – TensorFlow, PyTorch, Scikit-learn, …
- … — *not limited to the above list*

Licensed software

- VSC or campus-wide license
  - e.g.: MATLAB, Mathematica, Maple, …
  - restrictions may apply if you don't work at UAntwerp
    - for external institutions (ITG, VITO) and companies

- Other restricted licenses
  - e.g.: VASP, Gaussian, …
    - typically paid for by research groups (or individual users)
    - sometimes just other license restrictions that must be respected
  - access controlled via *group membership*
    - talk to the owner of the license first
    - request group membership via the VSC account page ("New/Join group")
    - the group moderator will grant or refuse access

Software installation and support

- Installed in **/apps/antwerpen**
  - preferably built and installed using **EasyBuild**
  - often multiple versions of the same package
- Additional software – *installed on demand*
  - system requirements should be met – *note: no Windows software*
  - provide building instructions (no rpm/deb packages)
    - is the software supported by EasyBuild?
  - commercial software must have a *cluster-use license*
  - assist in testing – we can't have expertise in all domains
- Limited (compilation) support
  - best effort, no code fixing
  - many packages are tested with only one compiler

Selecting software

- Using **modules**
  - dynamic software management
  - no version conflicts
  - automatically loads required dependencies
  - sets environment variables
    - generic – `$PATH`, `$LD_LIBRARY_PATH`, …
    - application-specific – `$PYTHONPATH`, …
    - EasyBuild related – `$EBROOT`…
- Module naming scheme

```
<name of software>/<version>[-<toolchain info>][-<additional info>]
```

  - toolchain = bundle of compiler + compatible MPI and math libraries
  - additional information: used to distinguish between versions

Toolchains

- **Toolchain** = bundle of compiler + compatible MPI and math libraries
  - `intel` – Intel & GNU compilers, Intel MPI and MKL libraries
  - `foss` – GNU compilers, Open MPI, OpenBLAS, FFTW, ...

- *Subtoolchains* — not including MPI or mathematical libraries
  - `gfbf` = GCC + FlexiBLAS + FFTW
  - `GCC` = GCCcore + binutils
  - `GCCcore` — GNU compilers only

- System toolchain – system compilers (installed as part of the OS)

- Refreshed yearly (actually, twice per year) → 2025a, 2024b, 2024a, 2023b, 2023a
  - offers more recent versions of the components (and of the software built with it)

Overview of common toolchains (and their component versions)

CalcUA modules

- Used to group software installed in the same time frame

CalcUA module	Software collection
`calcua/2025a`	version 2025a of the *toolchain compiler* modules + software built with them
`calcua/system`	software built with *system compilers*
`calcua/x86_64`	software installed from *binaries* (x86_64)
`calcua/all`	all currently available software (all of the above)

- Currently available versions of the toolchain compiler modules
  - 2025a, 2024a, 2023a: mostly foss, but also intel

- *Good practice: always load a* `calcua` *module first!*

Using modules

- One command for searching, loading and unloading modules: **`module`**

`$ module av openfoam`	Show/search *available* modules • depends on currently loaded `calcua` module • *case-insensitive*
`$ module spider openfoam`	Show/search all *installed* modules • also includes *extensions* (e.g., Python packages, …)
`$ module spider openfoam/11-foss-2023a`	Display additional information about a specific module • shows which calcua modules provide it
`$ module load OpenFOAM/11-foss-2023a`	**Load** a *specific* version of a module • advise: explicitly specify name & version • *case-sensitive*
`$ module list`	List all *loaded* modules (in the current session)

Best practices for using modules

```
$ module purge
```

Unload *all* modules – start from a clean environment
- removal of a sticky module using `--force`

```
$ module load calcua/2023a
```

Load appropriate `calcua` module first
- makes the modules available (here, from 2023a)

```
$ module load
  OpenFOAM/11-foss-2023a
```

Load the modules you want to use
- advise: explicitly specify name & version

- *Advice: do not load modules in your .bashrc*
  - consider using module collections instead – subcommands: `save`, `savelist`, `describe`, `restore`

- Module system basics
- User's Tour of the Module Command

Hands-on

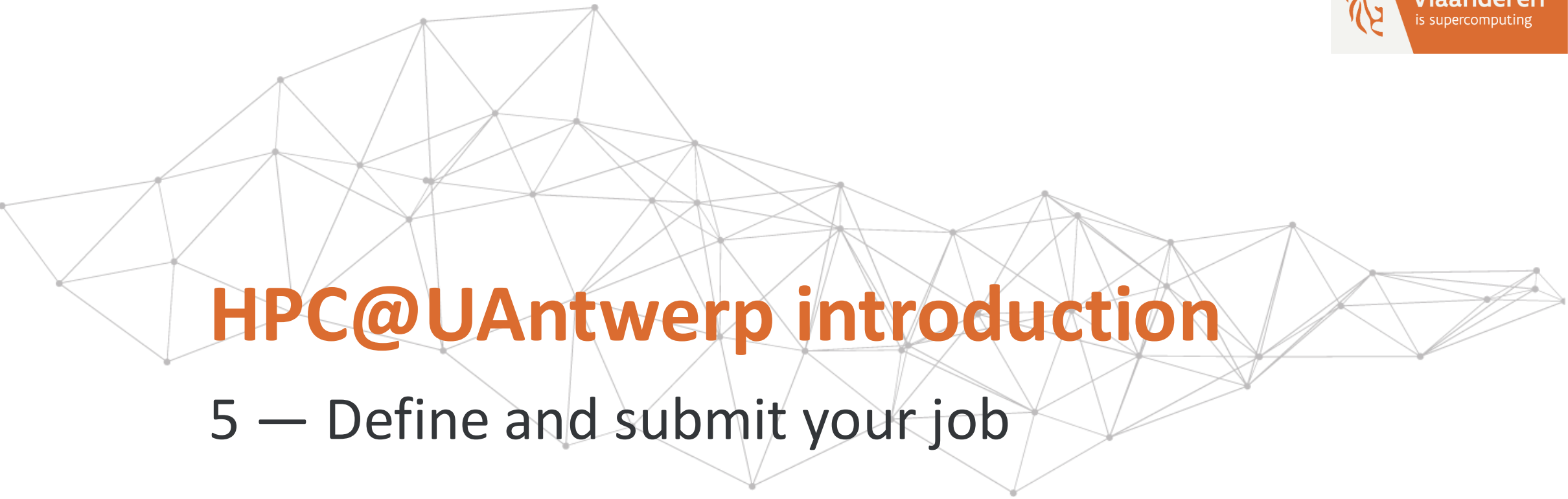
- Which software are you going to use?
  - can you find which versions we have?
  - if we do not have it, is it supported by EasyBuild?
    - yes → let us know
    - no → look for instructions & let us know
- Use our advice to load the modules
  - start from a clean environment
  - load an appropriate `calcua` module
  - load the module you want to use
- Try out saving and restoring a module collection

Summary — Select software & build your environment

- Installed software is isolated from the rest of the system using **modules**

  ```
  $ module load R/4.3.2-gfbf-2023a
  ```

- The modules are grouped in different **CalcUA modules**
  - `calcua/all` is loaded by default
- You can gain access to licensed software by requesting group membership in the VSC account page
- You can request additional software



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5 — Define and submit your job

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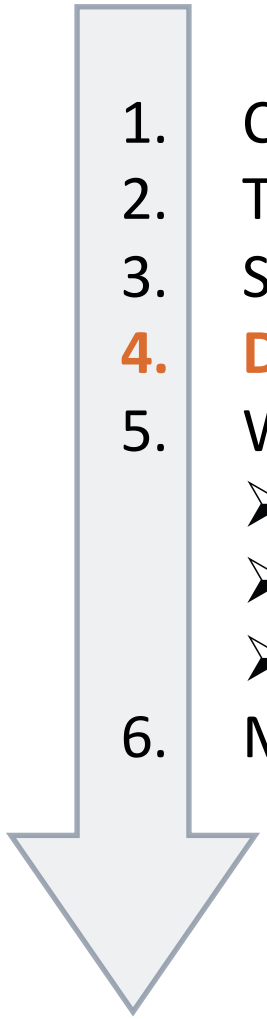
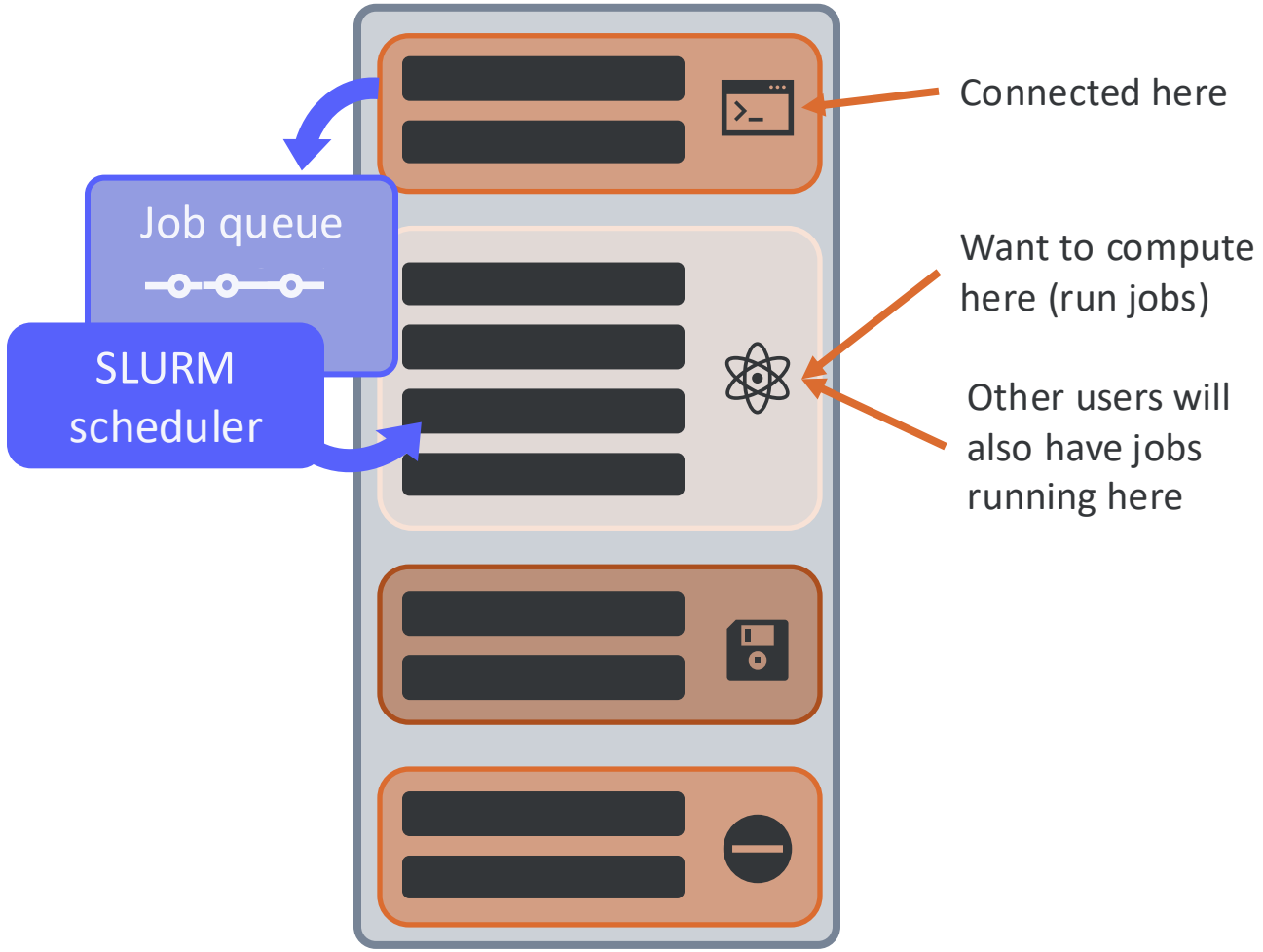
A typical workflow



1. Connect to the cluster
2. Transfer your files to the clusters
3. Select the software and build your environment
4. **Define and submit your job**
5. Wait while
   - ➢ your job gets scheduled
   - ➢ your job gets executed
   - ➢ your job finishes
6. Move your results

Running batch jobs

- Running computations → **batch jobs**
  - script with resource specifications
- Submitted to a queueing system
  - managed by a resource manager
- Next job selected by a scheduler
  - in a fair way – *fair share*
  - based on available resources
  - & scheduling policies
- Remember:
  - a cluster is a shared infrastructure
  - jobs might not start immediately



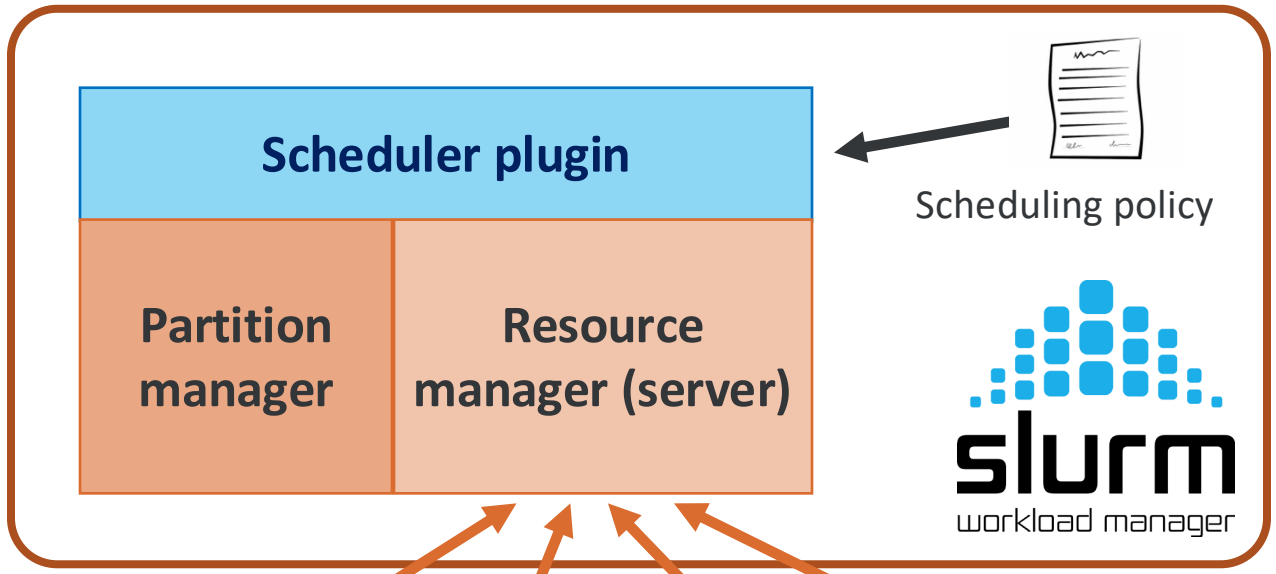
Job submission workflow – Behind the scenes

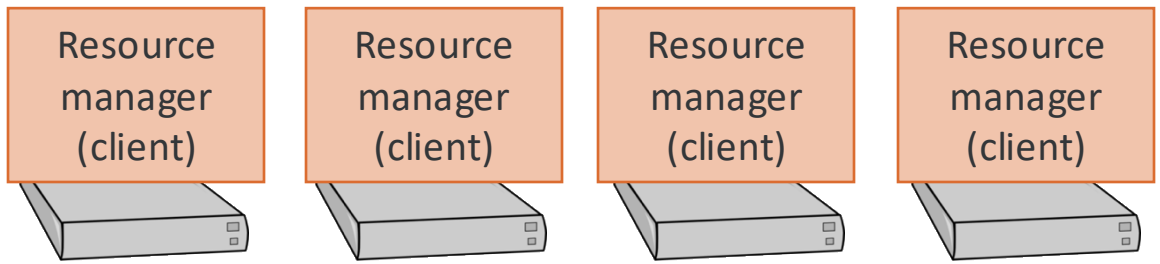
```
#!/bin/bash
#SBATCH -o stdout.%j
#SBATCH -e stderr.%j
module purge
module load calcua/all
module load MATLAB

matlab -r fibo
```

Job script

Users

Submit jobs
Query the cluster





Job script example

- Start with *shebang* line
- Request resources + give instructions
  - first block
  - start with **#SBATCH**
    - these look like comments to bash
- Load relevant modules
  - *build a suitable job environment*
- Actual computation commands

```
#!/bin/bash

#SBATCH --ntasks=1 --cpus-per-task=1
#SBATCH --time=0:10:00
#SBATCH --account ap_course_hpc_intro
#SBATCH --partition=zen2
#SBATCH --output stdout.%j
#SBATCH --error stderr.%j

module purge
module load calcua/2024a
module load Python/3.12.3-GCCcore-13.3.0

python pi.py
```

Important Slurm concepts

Node	Compute node
Core	Physical core (in physical cpu)
CPU	Virtual core – *hardware thread* • on the CalcUA clusters, hyperthreading is disabled → **CPU = Core**
Partition	Group of nodes with job limits and access controls – *aka job queue*
Job	Submitted job script — *resource allocation request*
Job step	Set of (possibly parallel) tasks within a job • the job script itself is a special step – the *batch job step* • e.g., a MPI application typically runs in its own job step
Task	Corresponds to a (single) Linux process, executed in a job step • a single task can not use more CPUs than available in a single node • e.g., for a MPI application, each rank (MPI process) is a task but a shared memory program is a single task

Slurm resource requests – Overview

Long option	Short option	Description
`--ntasks=<number>`	`-n <number>`	Number of tasks
`--cpus-per-task=<ncpus>`	`-c <ncpus>`	Number of CPUs per task
`--mem-per-cpu=<amount><unit>`		Amount of memory per CPU
`--time=<time>`	`-t <time>`	Time limit (wall time)
`--account=<ap_proj>`	`-A <ap_proj>`	Project account to use
`--partition=<pname>`	`-p <pname>`	Partition to submit to
`--switches=<count>`		Max count of leaf switches
`--job-name=<jobname>`	`-J <jobname>`	Name of the job
`--output=<outfile>`	`-o <outfile>`	Redirect stdout
`--error=<errfile>`	`-e <errfile>`	Redirect stderr
`--mail-type=<type>`		Event notification (start, end, …)
`--mail-user=<email>`		Email address

Slurm resource requests – Tasks & CPUs per task

Long option	Short option	Job environment variable	Description
`--ntasks=<number>`	`-n <number>`	`SLURM_NTASKS` (if set)	Number of tasks
`--cpus-per-task=<ncpus>`	`-c <ncpus>`	`SLURM_CPUS_PER_TASK` (if set)	Number of CPUs per task

- Specify number of (parallel) tasks and CPUs (cores) per task
  - Task = single process (runs within a single node)
  - CPUs per task → number of computational threads for a task
- *Note: CPUs per task can never exceed the number of cores per node*
- If not set, **default = 1 task & 1 CPU**

Slurm resource requests – Memory per CPU

Long option	Job environment variable	Description
`--mem-per-cpu=<amount><unit>`	`SLURM_MEM_PER_CPU` (in megabytes)	Amount of memory per CPU

- Memory per CPU – not per task
  - `unit` = kilobytes (k), megabytes (`m`) or gigabytes (g)
  - `amount` = integer — `3.75g` is invalid, use `3840m` instead
- If not set, **default = maximum available memory** *per requested CPU*
  - depends on node or partition setting
- *Note: if requesting more than maximum available per CPU → number of CPUs will be increased*
- Note: on CalcUA clusters, per node 16 GB is reserved for the OS and file system buffers
  - e.g., on a Vaughan compute node with 256 GB of (installed) memory, the default value is `3840m` – calculated from (256 GB - 16 GB) / 64 CPUs = 240 / 64 = **3.75GB = 3840 MB (per core)**

Slurm resource requests – Wall time

Long option	Short option	Job environment variable	Description
`--time=<time>`	`-t <time>`	`SLURM_JOB_START_TIME` `SLURM_JOB_END_TIME`	Time limit = ***wall time***

- Formats : `mm` | `mm:ss` | `hh:mm:ss` | `d-hh` | `d-hh:mm` | `d-hh:mm:ss`
  - d = days, hh = hours, mm = minutes, ss = seconds
- Maximum time limit on the CalcUA clusters
  - compute nodes: 3 days (Vaughan, Leibniz), 7 days (Breniac)
  - GPU nodes: 1 day
- *Wall time exceeded → job will be killed*
- *Wall time > maximum → job will not start*
- If not set, **default = 1 hour**

Slurm resource requests – Project account

Long option	Short option	Job environment variable	Description
`--account=<ap_proj>`	`-A <ap_proj>`	`SLURM_JOB_ACCOUNT`	Project account to use

- Required to specify a **project account** at CalcUA clusters
  - accounting for both compute (jobs) and storage (files)
  - *ask your supervisor or project account manager to get access*
  - use an appropriate account according to the project

- Show accounts you have access to: `myprojectaccounts`
  - all project accounts start with **ap_**
  - during this course → `ap_course_hpc_intro`

Accounting @ CalcUA (slides & video)

Slurm resource requests – Partitions

Long option	Short option	Job environment variable	Description
`--partition=`*<pname>*	`-p` *<pname>*	`SLURM_JOB_PARTITION`	Partition to submit to

- Partition = group of nodes
  - access controls and scheduling policies — e.g.: restrict access to a limited group of users
  - job defaults & resource limits – e.g.: def/max mem per CPU, max time limit, def CPUS per GPU
- If not set, use the **default partition defined per cluster**
  - *note: job does not get automatically assigned to the optimal partition*

UAntwerp Tier-2 Infrastructure – available partitions per cluster + resource limits

CalcUA clusters – Partitions and node information

Cluster	Partition	#	Specifications	CPU – GPU	Mem per CPU	Max WT
Vaughan	**zen2**	152	AMD Zen 2, 256 GB RAM	64 CPU	3.75 GiB – `3840m`	3 days
	zen3	28	AMD Zen 3, 256 GB RAM	64 CPU	3.75 GiB – `3840m`	
	zen3_512	12	AMD Zen 3, 512 GB RAM	64 CPU	7.75 GiB – `7936m`	
	ampere_gpu	1	Zen 2, NVIDIA Ampere GPUs	4 GPU – 64 CPU	3.75 GiB – `3840m`	1 day
	arcturus_gpu	2	Zen 2, AMD Arcturus GPUs	2 GPU – 64 CPU	3.75 GiB – `3840m`	
Leibniz	**broadwell**	144	Intel Broadwell, 128 GB RAM	28 CPU	4 GiB – `4096m`	3 days
	broadwell_256	8	Intel Broadwell, 256 GB RAM	28 CPU	8,5 GiB – `8704m`	
	pascal_gpu	2	Broadwell, NVIDIA Pascal GPUs	2 GPU – 28 CPU	4 GiB – `4096m`	1 day
Breniac	**skylake**	23	Intel Skylake, 192 GB RAM	28 CPU	6.29 GiB – `6436m`	7 days

- **bold** = default partition for the corresponding cluster

Hands-on

- And now it's **time to run your first job** – *finally!*
  - *start by cloning our repository for this course*

    ```
    git clone https://github.com/hpcuantwerpen/intro-hpc
    ```

- Create a small job script which
  - uses the correct project account – *for this course*
  - needs 1 core, has a wall time of 10 minutes, and will run on the zen2 partition
  - loads the module `vsc-tutorial/202203-intel-2024a` – *according to our advice*
  - executes a "hello world" script by using the command: `serial_hello`

- Submit your first job
  - submit the job – use **sbatch** → you get a *job id*
  - be patient, the job will start soon – check the job status using **squeue**
  - look at what happens – e.g.: which files are generated?

Slurm resource requests – Faster communication

Long option	Description
`--switches=1`	Request all nodes to be connected to a single switch

- Node communication through network switches
  - Nodes are grouped on *edge* switches which are connected by *top* switches
    - hence communication/traffic between two nodes passes through either 1 or 3 switches
- Some programs are latency-sensitive – e.g.: GROMACS
  - will run much better on nodes which are all connected to a single (edge) switch
- *Note: using this option might increase your waiting time*

Slurm resource requests – Exclusive node access

Long option	Description
`--exclusive`	Request exclusive access to the node for the job

- Nodes are shared resources
  - *if you don't request all cores, remaining cores might be used by another user*
  - *if you submit multiple jobs, those might end up on the same or on different nodes*
- Sometimes it is better to request exclusive access to the compute nodes
  - because jobs influence each other (L3 cache, memory bandwidth, communication channels, ….)
  - prevents sharing of allocated nodes with other jobs – even from the same user
- *Be aware, you will be charged for a full node*

Slurm resource requests – Number of nodes

Long option	Short option	Job environment variable	Description
`--nodes=<number>`	`-N <number>`	`SLURM_JOB_NUM_NODES`	Number of nodes

- For each task, all of the CPUs for that task are allocated on a single compute node
  - but different (parallel) tasks might end up on either the *same* or *different* compute nodes
  - depends on what is already running on these nodes — from you or another user
- *Advice: bundle tasks from the same job on as few nodes as possible*
  - to make the communication latency between tasks as small as possible
- Specify the number of nodes the job may use
  - tell the scheduler how many nodes it needs to allocate for the job
  - note: also possible to specify a min/max number of nodes using `--nodes=<min>-<max>`

Non-resource-related options – Job name

Long option	Short option	Job environment variable	Description
`--job-name=<jobname>`	`-J <jobname>`	`SLURM_JOB_NAME`	Name of the job

- Assign a name to your job – the *job name*
  - job name can be used when defining the output and error files

- If not given, the **default name = name of the batch job script**
  - or “sbatch” if read from standard input

Non-resource-related options – Redirect stdout / stderr

Long option	Short option	Description
`--output=<outfile>`	`-o <outfile>`	Redirect stdout
`--error=<errfile>`	`-e <errfile>`	Redirect stderr

- By **default = redirect both stdout and stderr** → **slurm-<jobid>.out**
  - that file is present as soon as the job starts and produces output
  - but delays may occur due to buffering or filesystem caches
- If only `--output` is given → redirect *both* stdout and *stderr* *to the same file*
- Possible to use *filename patterns* to define the filename
  - examples: **%x** for the job name, **%j** for job id, …

Filename patterns

Non-resource-related options – Mail notifications

Long option	Description
`--mail-type=<type>`	Event notification (start, end, …)
`--mail-user=<email>`	Email address

- The scheduler can send you a mail when a job begins (starts), ends or fails (gets aborted)
  - `type = BEGIN | END | FAIL | ALL | TIME_LIMIT_xx`
- **default email address** = linked to your VSC-account

The job runtime environment

- On UAntwerp clusters, we only set a minimal environment for jobs by default
  - equivalent to exporting only these environment variables

```
--export=HOME,USER,TERM,PATH=/bin:/sbin
```

  - *hence you need to (re)build a suitable environment for your job – using modules*

- Other available environment variables include
  - `VSC_*` — for user directories, but also for cluster/os/architecture
  - `EB*` + module specific variables – defined by loading modules
  - `SLURM_*` variables – set by Slurm (next slide)

The job environment

The job runtime environment

- Slurm defines several variables when a job is started
  - these can be used when calling programs – e.g.: to pass the number of available CPUs
  - *some are only present if explicitly set*

Environment variable	Explanation
SLURM_SUBMIT_DIR	The directory from which sbatch was invoked
SLURM_JOB_ACCOUNT	Account name selected for the job
SLURM_JOB_NUM_NODES	Total number of nodes for the job
SLURM_JOB_NODELIST	List of nodes allocated to the job
SLURM_JOB_CPUS_PER_NODE	CPUs available to the job on this node
SLURM_TASKS_PER_NODE	Number of tasks to run on this node

Output environment variables

Summary — Define & submit your job

jobscript.sh

```
#!/bin/bash
#SBATCH --ntasks=1 --cpus-per-task=1
#SBATCH --time=0:10:00
#SBATCH --account ap_course_hpc_intro
#SBATCH --output stdout.%j
#SBATCH --error stderr.%j
module purge
module load calcua/2024a
module load R/4.3.2-gfbf-2023a
...
```

- Computations (batch jobs) are scheduled by **Slurm** to run on the compute nodes
- In your jobscript, you **request** the appropriate **resources**:
  - number of cores/ tasks,
  - memory,
  - partition,
  - project account,
  - wall time, …

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X — Using the command line

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SSH access — Required software

- **Windows**
  - SSH client included in latest versions of Windows 10 or above
    - check if present in Windows Settings > System > Optional features
  - optional: use Windows Subsystem for Linux (WSL)
    - install and use a Linux distribution of your choice
    - now also supports running Linux GUI apps (X11 and Wayland)
  - optional: use Windows Terminal (available via the Microsoft Store)
    - choose between Command Prompt, PowerShell, and bash (via WSL)
  - MobaXterm combines a SSH/SFTP client, X server and VNC server in one
  - PuTTY used to be a popular GUI SSH client

SSH access — Required software

- **macOS**
  - SSH client included
  - Terminal app (built-in) or iTerm2
  - for graphical applications (X11), use XQuartz
  - optional: Homebrew
    - allows to install Linux commands
    - can also install applications
  - remark: macOS is based on BSD (Unix)
    - (BSD variants of) commands may behave differently

- **Linux**
  - SSH client included
  - choice of terminal and shell
  - supports graphical applications

SSH access — Public/private key pairs

- Communication with the cluster happens through **SSH** (Secure SHell)
  - Protocol to log in to a remote computer, transfer files (**SFTP**), …
  - uses public/private key pairs

private key

`/home/<username>/.ssh/id_rsa`

Keep safe!

public key

`/home/<username>/.ssh/id_rsa.pub`

Upload to VSC account page

SSH access — Public/private key pairs

- Create a public/private key pair
  - create RSA key pair (at least 4096 bits)

```
$ ssh-keygen -t rsa -b 4096
```

  - note: on Windows, when using PuTTYgen key generator
    - use PuTTY key format 2 in latest version
    - Convert the public key to OpenSSH format

- Upload public key → VSC account page
  - web-based registration procedure

SSH access — Connect to the cluster

- You need:
  - VSC account name: **vsc2xxxx**
  - Hostname of a login node
  - Private/public key pair
    (upload public key once)

- Restricted public access
  - outside of Belgium: use **VPN**
    - vpn.uantwerpen.be
    - Instructions on Pintra (staff)

      My Subsites > Department ICT
      > ICT Guide > Remote working – VPN

      or Studentportal (students)

      Dashboard > ICT > Network > VPN

Cluster	Hostname of login node
Vaughan	login-vaughan.hpc.uantwerpen.be
Vaughan (indiv. login nodes)	login1-vaughan.hpc.uantwerpen.be login2-vaughan.hpc.uantwerpen.be
Leibniz	login-leibniz.hpc.uantwerpen.be **login.hpc.uantwerpen.be**
Leibniz (indiv. login nodes)	login1-leibniz.hpc.uantwerpen.be login2-leibniz.hpc.uantwerpen.be
Leibniz (vis. node)	viz1-leibniz.hpc.uantwerpen.be
Breniac	login-breniac.hpc.uantwerpen.be

SSH access — Connect to the cluster

- Login via secure shell
  - if your private key has the standard filename (`~/.ssh/id_rsa`)

```
$ ssh vsc2xxxx@login.hpc.uantwerpen.be
```

  - otherwise, explicitly specify the filename

```
$ ssh -i ~/.ssh/id_rsa_vsc vsc2xxxx@login.hpc.uantwerpen.be
```

Text-mode access using OpenSSH

SSH access — Using an SSH configuration file

```
Host *
  ServerAliveInterval 60

Match final User vsc2xxxx
  IdentityFile ~/.ssh/id_rsa_vsc

Host calcua
  User vsc2xxxx
  HostName login.hpc.uantwerpen.be
  ForwardAgent yes
  ForwardX11 yes
```

→ for all hosts
- (try to) keep the connection alive

→ when connecting as user `vsc2xxxx`
- use this private key

→ create a shorthand "`calcua`"
- connect as user `vsc2xxxx`
- use login node `login.hpc.uantwerpen.be`
- use agent forwarding (for subsequent ssh calls (`-A`))
- use X11 forwarding (for visualisation (`-X`))

➢ Put this file in `~/.ssh/config` and then you can connect using: `ssh calcua`

SSH config

SCP/SFTP access — Transfer your files

- For simple file transfers: secure copy (**SCP**)
  - copy from your local computer to the cluster

```
$ scp file.ext vsc2xxxx@login.hpc.uantwerpen.be:
```

  - copy from the cluster to your local computer

```
$ scp vsc2xxxx@login.hpc.uantwerpen.be:file.ext .
```

- Need more features (e.g.: file browsing, resuming transfers, …): use **SFTP**
  - command-line: `sftp`
  - any graphical sftp file manager of your choice

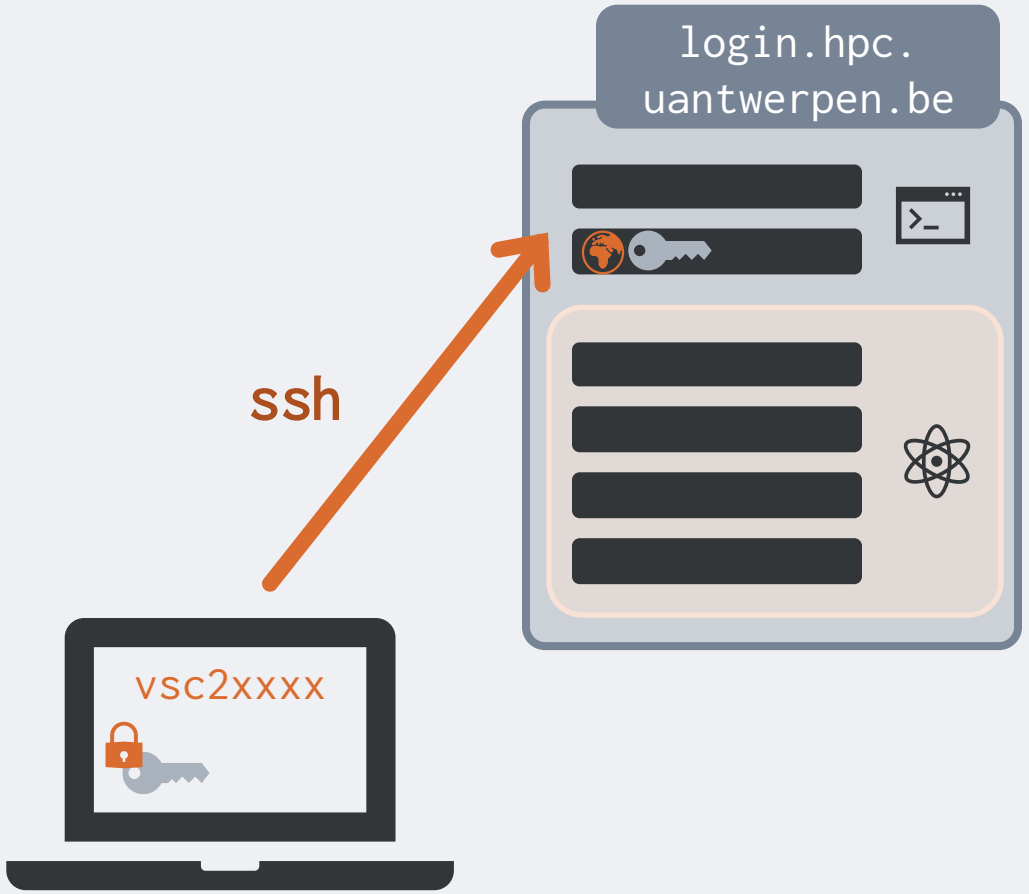
- For large file transfers, we recommend **Globus**

Data transfer on external computers

Hands-on

- Install the required software
- Create your VSC account
  - create a public/private key pair
  - upload your public key
- Login to a CalcUA cluster via **ssh**
- Copy a file from CalcUA to your computer using **scp**
- Create a SSH configuration file
  - *feel free to choose your own shorthand name*
  - login using the shorthand name

Summary — SSH access



- You can connect directly to the cluster's **login nodes**, not the compute nodes
- To connect using `ssh`, you need:
  - your **VSC account** name
  - the **hostname** of the login node
  - your **private key**
- Your private key is private, keep it safe!

Globus – Command line interface

Setup

- `$ module load Globus-CLI/3.34.0-GCCcore-13.3.0`
- `$ globus login`
  - paste url in browser, follow instructions & copy code back to terminal
- `$ globus endpoint search "VSC UAntwerpen Tier2 filesystems"`
- `$ Tier2Antwerp=6a13242d-6506-4b3d-a49c-ac981b35ab7d`
  - you can add these as environment variables to ~/.bashrc
- `$ globus ls $Tier2Antwerp`
  - first time access error: "`Missing required data_access consent`"
  - `$ globus session consent "urn:globus:auth:scope:transfer.api.globus.org:all [*https://auth.globus.org/scopes/<COLLECTION_ID>/data_access]"`

Globus – Command line interface

Transfer

- `$ module load Globus-CLI/3.34.0-GCCcore-13.3.0`
- `$ globus endpoint search --filter-scope my-endpoints <name>`
  - `$ Tier2Antwerp=6a13242d-6506-4b3d-a49c-ac981b35ab7d`
  - `$ MyPC=…`
- `$ globus ls $Tier2Antwerp:/scratch/antwerpen/xxx/vsc2xxyy/`
- `$ globus transfer $Tier2Antwerp:path/to/data/on/uantwerp/tier2 \`
  `$MyPC:path/to/data/on/your/pc/ --label "test_transfer”`

Globus Command Line Interface (CLI) — Reference

OneDrive – Command line interface

- OneDrive Client for Linux
  - alternative: UAntwerp OneDrive collection for Globus — *not yet available*

Setup

- `$ onedrive`
  - copy url in browser, follow instructions, copy response url back to terminal
  - use Chrome if you encounter issues
- Configure a directory to be synchronized:
  - `$ mkdir -p $VSC_DATA/onedrive/calcua-sync`
  - `$ config=~/.config/onedrive/config`
  - `$ echo sync_dir = \"$VSC_DATA/onedrive\" > $config # set onedrive directory`
  - `$ echo 'skip_symlinks = "true"' >> $config # do not sync symlinks`
  - `$ echo 'skip_dotfiles = "true"' >> $config # do not sync hidden files`

OneDrive – Command line interface

- You don't want to sync your entire OneDrive
  `~/.config/onedrive/sync_list` defines which files and directories to sync
  - `$ echo calcua-sync >> ~/.config/onedrive/sync_list`
  - supports excluding and/or including files and/or directories (see example)
- After changing `sync_list`:
  - `$ onedrive --resync --sync --verbose --dry-run`

Transfer

- Perform a synchronization:
  - `$ onedrive --sync --verbose`

Using the client

`~/.config/onedrive/sync_list`

```
# exclusions should be listed first
!/Documents/secret/ # exclude this directory, otherwise included in next line
/Documents/ # include Documents folder in OneDrive root
Results/ # include Results folder anywhere in OneDrive
Reports/*.pdf # include all .pdf files in a Reports folder anywhere in OneDrive
```

Part 2 — Sneak preview

- In **Part 1**, you learned how to
  - connect to the cluster and transfer your files
  - use modules and setup your job environment
  - properly specify your resource requests
  - write and submit your job scripts

- In **Part 2**, you will learn
  - more about the Slurm commands and how to use them
  - the different types of multi-core parallel jobs
  - how to organize your job workflows
  - running large number of jobs
  - and some best practices

HPC@UAntwerp introduction

Ine Arts, Franky Backeljauw, Michele Pugno, Robin Verschoren

Version Fall 2025 — Part 2

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- sstat and sacct : information about jobs
- sinfo : get an overview of the cluster and partitions
- scontrol : view Slurm configuration and state
- salloc : create a resource allocation

7. Multi-core parallel jobs

- Why parallel computing?
- Types of parallel computing
- Running a shared memory job – Multithreading (OpenMP)
- Running a distributed memory job – MPI
- Running a hybrid OpenMP/MPI job
- Job monitoring

8. Multi-job submission

- Running a large batch of small jobs
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9. Installing your own software

- Installing your own software and packages
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- Running interactive applications on the compute nodes
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X. Extra topics

- Organizing job workflows

Final notes

HPC@UAntwerp introduction

6 — Slurm commands

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Slurm commands – Overview

	Command	Description
	`sbatch`	Submit a batch script
	`squeue`	Check the status of your jobs
	`scancel`	Cancel a job
	`srun`	Run parallel tasks – start an interactive job
	`sstat`	Information about *running* jobs
	`sacct`	Information about (terminated) jobs
	`sinfo`	Get an overview of the cluster, partitions and nodes
	`scontrol`	View current Slurm configuration and state
	`salloc`	Create a resource allocation

sbatch — Submit a batch script

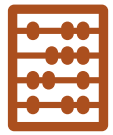
- `sbatch <sbatch arguments> jobscript <arguments of the job script>`
  - does not wait for the job to start or end
  - can also read the job script from stdin instead
- What sbatch does:
  - submits the job script to the selected partition (aka *job queue*)
  - returns `Submitted batch job <jobid>`
- What Slurm does – *behind the scenes*
  - creates an allocation when resources become available
  - creates batch job step in which it runs the batch script

sbatch — Submit a batch script

- To pass resource (and non-resource) requests
  - add #SBATCH comment lines at the beginning of your job scripts
  - use environment variables beginning with SBATCH_
    - followed by the name of the matching command line option
    - can be useful if you have access to only one project account
    - overrules #SBATCH lines
  - on the command line as options to sbatch
    - overrules both #SBATCH and SBATCH_*

sbatch manual page

squeue — Check the status of your jobs



- `squeue` checks the status of your *own* jobs in the job queue

```
$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             26170      zen2     bash vsc20259  R       6:04      1 r1c02cn3.vaughan
```

  - ST = state of the job

ST	Explanation
PD	Pending – waiting for resources
CF	Configuring – nodes becoming ready
R	Running
CD	Successful completion – exit code zero

ST	Explanation
F	Failed job – non-zero exit code
TO	Timeout – wall time exceeded
OOM	Job experienced out-of-memory error
NF	Job terminated due to node failure

squeue manual page – job state codes

squeue — Check the status of your jobs

- `squeue` checks the status of your *own* jobs in the job queue

```
$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             26170      zen2     bash vsc20259  R       6:04      1 r1c02cn3.vaughan
```

  - **NODELIST(REASON)** = reason why a job is waiting for execution

NODELIST(REASON)	Explanation
Priority	There are one or more higher priority jobs in the partition
QOSMaxNodePerUserLimit	The limit on the maximum number of nodes per user is exceeded
AssocMaxJobsLimit	The limit on the number of running jobs for each user has been reached
JobHeldAdmin	The job is held by an administrator

job reason codes

`scancel` — Cancel a job

- `scancel <jobid>` cancels a single job + all its job steps (if already running)
  - cancel a specific job step: `scancel <jobid>.<stepid>`
    - *e.g., if you suspect a job step hangs, but you still want to execute the remainder of the job script to clean up and move results*
  - cancel a (sub)job of a job array: `scancel <jobid>_<arrayid>`

- Some other possibilities
  - `--state <state>` or `-t <state>` : cancel only jobs with given state
    - `<state>` = `pending`, `running`, or `suspended`
  - `--partition <part>` or `-p <part>`: cancel only jobs in given partition

scancel manual page

`srun` — Run parallel tasks

- `srun` *"Swiss Army Knife"* to create & manage (parallel) tasks within a job
  - in Slurm terminology: it creates a job step that can run one or more parallel tasks
  - run multiple jobs steps *simultaneously*, each using a part of the allocated resources
  - *the better way of starting MPI programs* – preferred over `mpirun` and `mpiexec`
    - usage will be shown through examples
  - run a command on all allocated nodes of a running job:

    ```
    srun --jobid <jobid> --overlap <command>
    ```

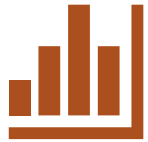
  - run a shell on the first allocated node of a running job:

    ```
    srun --jobid <jobid> --interactive --pty bash
    ```

  - alternatively, use **ssh** to log into any allocated node of a running job
    - but only possible as long as the job is running

srun manual page

sstat — Information about running jobs



- `sstat -j <jobid>[.<stepid>]` shows real-time information about a job or job step
  - it is possible to specify a subset of fields to display using the `-o`, `--format` or `--fields` option.
- Get an idea of the load balancing (for an MPI job)

```
$ sstat -a -j 12345 -o JobID,MinCPU,AveCPU
      JobCPU     MinCPU     AveCPU
------------ ---------- ----------
12345.extern  00:00.000  00:00.000
12345.batch   00:00.000  00:00.000
12345.0        22:54:20   23:03:50
```

  - shows the minimum and average amount of *consumed* CPU time for all job steps
    - interpretation: here, step 0 is an MPI job, and we see that the minimum CPU time consumed by the task is close to the average, which indicates that the job is running properly and that the load balance is ok

sstat — Information about running jobs

- Checking memory usage

```
$ sstat -a -j 12345 -o JobID,MaxRSS,MaxRSSTask,MaxRSSNode
       JobID     MaxRSS MaxRSSTask MaxRSSNode
------------ ---------- ---------- ----------
12345.extern
12345.batch       4768K          0 r1c06cn3.+
12345.0         708492K         16 r1c06cn3.+
```

  - provides a snapshot of the job's real memory usage – RSS = Resident Set Size
    - gives an insight into how much of the requested memory the job is actively using
    - interpretation: the largest process in the MPI job step is consuming roughly 700MB at this moment, and it is task 16 and running on compute node r1c06cn3.vaughan

sstat manual page

sacct — Information about (terminated) jobs

- `sacct` shows information kept in the *job accounting database*
  - e.g.: job start/end times, resource usage, job status, user/account details, …
  - useful for monitoring, billing, performance analysis, …
  - note: for running jobs the information may enter only with a delay

```
$ sacct -j 12345
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
12345        NAMD-S-00+       zen2 antwerpen+         64  COMPLETED      0:0
12345.batch       batch            antwerpen+         64  COMPLETED      0:0
12345.extern     extern            antwerpen+         64  COMPLETED      0:0
12345.0           namd2            antwerpen+         64  COMPLETED      0:0
```

sacct — Information about (terminated) jobs

- Retrieving job details
  - get an overview for jobs in a given time range

    ```
    sacct -S <start-datetime> -E <end-datetime> -X
    ```

    - datetime format: `YYYY-MM-DD[THH:MM[:SS]]` (other formats possible)
  - get (all) the details of a given job — module load Miller

    ```
    sacct -j <jobid> -o ALL -XP | mlr --c2x --ifs='|' cat
    ```

  - get the batch script of a given job

    ```
    sacct -j <jobid> -B
    ```

sacct manual page

`sinfo` — Get an overview of the cluster

- `sinfo` shows information about the partitions and their nodes in the cluster

```
$ sinfo
PARTITION     AVAIL  TIMELIMIT  NODES  STATE NODELIST
zen2             up 3-00:00:00     38    mix r1c01cn1.vaughan, ...
zen2             up 3-00:00:00    112  alloc r1c01cn2.vaughan, ...
zen2             up 3-00:00:00      1   idle r4c05cn2.vaughan
zen3             up 3-00:00:00     24  idle~ r6c01cn1.vaughan, ...
broadwell        up 3-00:00:00      2  down~ r2c08cn1.leibniz, ...
ampere_gpu       up 1-00:00:00      1   idle nvam1.vaughan
```

  - show number of node is state allocated / mixed / idle / down
  - note: ~ = the node is in powersave mode

`sinfo` — Get an overview of the cluster

- Show info *per node*

```
$ sinfo -N -l -n r6c01cn4.vaughan,r1c02cn3.leibniz,amdarc2.vaughan
NODELIST          NODES    PARTITION       STATE CPUS    S:C:T MEMORY
amdarc2.vaughan       1 arcturus_gpu        idle 64     2:32:1 245760
r1c02cn3.leibniz      1    broadwell   allocated 28     2:14:1 114688
r6c01cn4.vaughan      1         zen3       idle~ 64     2:32:1 245760
```

  - **`MEMORY`** = *total* amount of memory that can be allocated on the node (in kilobytes)
  - **`S:C:T`** = structure of the node → sockets / cores / (hardware) threads

↗ sinfo manual page

`scontrol` — View Slurm configuration and state

- `scontrol` view Slurm configuration and state

- Show information about:
  - jobs: `scontrol -d show job <jobid>`
    - shows `CPU_IDs` of CPUs assigned to the job
  - partitions: `scontrol show part [<part>]`
  - Slurm configuration: `scontrol show config`

- Inside a job script to:
  - get a list of node names one per line: `scontrol show hostnames`
    - `$SLURM_JOB_NODELIST` contains the same list but separated by commas

scontrol manual page

`salloc` — Create a resource allocation

- `salloc` creates a resource allocation

- What `salloc` does – *behind the scenes*
  - requests the resources and waits until they are allocated
  - then start a shell on the node where you executed `salloc` – usually the login node
  - afterwards, releases the resources

- *Important*: *the shell is not running on the allocated nodes!*
  - but, from the shell, you can start job steps on the allocated resources using **`srun`**

salloc manual page

Hands-on

- Given the incomplete job script `matrix.slurm`, which compiles and runs `matrix_multiply.c`
  - make these changes to the job script
    - add the project account to the jobscript – use `ap_course_hpc_intro`
    - request 1 task with 10 cores
    - change the output and error formats to be `<jobname>.<jobid>.out`
      - *remember:* replace `<jobname>` and `<jobid>` by the proper *filename pattern*
    - send yourself an email when the job is finished
    - add a 300 second sleep at the end of the script – so it stays in the queue for a while longer
  - submit the jobscript
    - while the job is running, try several of the Slurm commands – `squeue` / `sstat` / `sacct`
    - what information is stored in the accounting database? – `sacct`

- Clone our repository: **`git clone`** `https://github.com/hpcuantwerpen/intro-hpc`

Summary — Slurm commands

- You can interact with the scheduler/resource manager Slurm through a series of commands
- You cannot go without:
  - `sbatch`: submit a batch script
  - `srun`: *Swiss army knife*
    - start a job step: run parallel tasks
    - start an interactive job
  - `sacct`: show information about (past) jobs

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7 — Multi-core parallel jobs

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Why parallel computing?

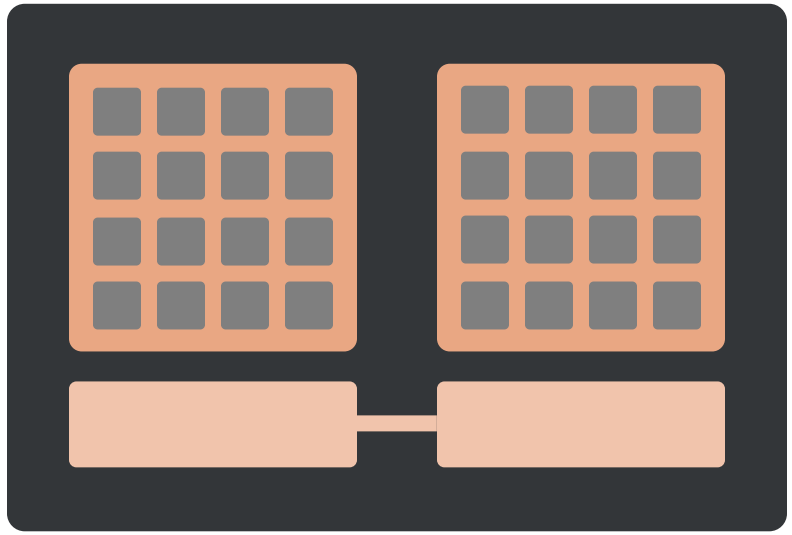
- Faster time to solution
  - distributing code over N cores
  - hope for a speedup by a factor of N
- Larger problem size
  - distributing your code over N nodes
  - increase the available memory by a factor N
  - hope to tackle problems which are N times bigger
- In practice
  - gain limited due to communication, memory overhead, sequential fractions in the code, …
  - optimal number of cores/nodes is problem-dependent
  - but, no escape possible – computers don't really become faster for *serial* code
- *Parallel computing is here to stay!*

Types of parallel computing

1. Multi**threading**
   - *shared memory*
   - OpenMP

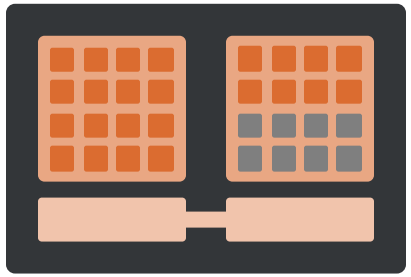
2. Multi**processing**
   - *distributed memory*
   - MPI

3. Hybrid
   - *combination*



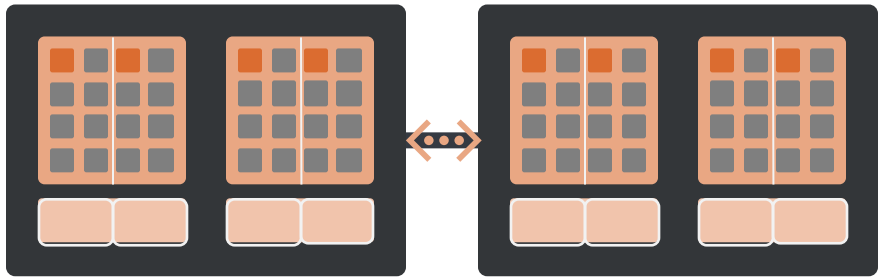
Types of parallel computing

1. Multi**threading**
   - *shared memory*
   - OpenMP



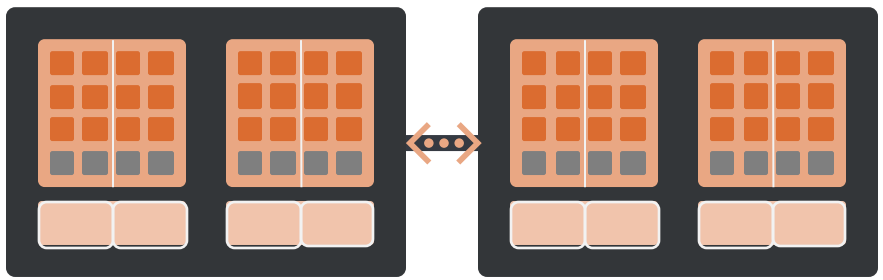
OpenMP software uses multiple or all cores in a **single** node
e.g. 24 threads within 1 node

2. Multi**processing**
   - *distributed memory*
   - MPI



MPI software can use (all) cores in **multiple** nodes
e.g. 8 tasks spread over 2 nodes

3. Hybrid
   - *combination*

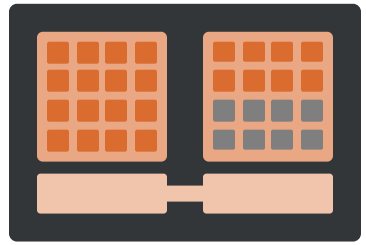


Hybrid OpenMP/MPI software
e.g. 6 threads per task
& 8 tasks over 2 nodes
(each task stays within 1 node)

Active core

Inactive core

Running a shared memory job – Multithreading



- **Shared memory job** = *single* task with multiple CPUs per task
  - all threads for the task run on within a *single* node
- Tell the program *how many threads* it can use
  - depends on the program - e.g.: for MATLAB, use `maxNumCompThreads(N)`
    - *note: autodetect usually only works if the program gets the whole node*
  - many OpenMP programs use the environment variable **`OMP_NUM_THREADS`**
    - Intel OpenMP recognizes Slurm CPU allocations
  - for MKL-based code/operations, use **`MKL_NUM_THREADS`** – instead of `OMP_NUM_THREADS`
  - for OpenBLAS (FOSS toolchain), use **`OPENBLAS_NUM_THREADS`**
- *Check the manual of the program you use!*
  - e.g., NumPy has several options (depending on how it was compiled)

Running a shared memory job – Multithreading

- OpenMP example script

generic-omp.slurm

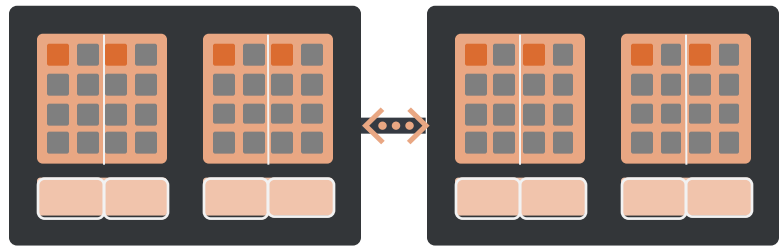
```
#!/bin/bash

#SBATCH --job-name=OpenMP-demo
#SBATCH -A ap_course_hpc_intro
#SBATCH --ntasks=1 --cpus-per-task=64          ← 1 task with 64 CPUs (so 64 threads)
#SBATCH --mem-per-cpu=2g                       ← 2 GB per CPU, so 128 GB total memory

module --force purge
module load calcua/2024a                       ← load the calcua module
module load vsc-tutorial/202203-intel-2024a    ← load vsc-tutorial – also loads the Intel
                                                  toolchain (for the OpenMP run time)
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK    ← set the number of (OpenMP) threads to use
export OMP_PROC_BIND=true                      ← threads stay on the core where they're created
omp_hello                                      ← run the program
```

Running a distributed memory job – MPI

- **Distributed memory job** = *several* tasks running in parallel
  - the tasks can be spread over *multiple (different)* nodes
  - communication → message passing interface (**MPI**)



- Every distributed memory program needs a *program starter*
  - some packages use system starter internally
  - mpirun works, but depends on variables set in the intel modules
    - so ensure to *properly load the module*!
  - the **preferred program starter for Slurm = srun**
    - knows how Slurm distributes processes
    - needs no further arguments if resources are correctly requested – tasks & CPUs per task
  - *Check the manual of the program you use!*
    - is there an option to explicitly set the program starter?

Running a distributed memory job – MPI

- (Intel) MPI example script

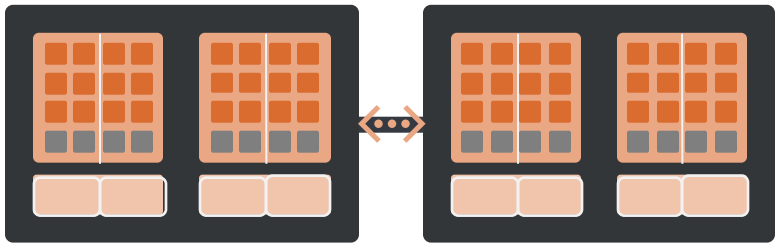
generic-mpi.slurm

```
#!/bin/bash

#SBATCH --job-name mpihello
#SBATCH -A ap_course_hpc_intro
#SBATCH --ntasks=128 --cpus-per-task=1          ← 128 MPI processes (uses 2 nodes on Vaughan, or
#SBATCH --mem-per-cpu=1g                            5 nodes on Leibniz/Breniac)

module --force purge
module load calcua/2024a                        ← load the calcua module
module load vsc-tutorial/202203-intel-2024a     ← load vsc-tutorial – also loads the Intel toolchain
                                                    (for the MPI libraries)
srun mpi_hello                                  ← run the MPI program – srun communicates
                                                    with the resource manager
```

Running a hybrid OpenMP/MPI job



- **Hybrid job** = combination of OpenMP and MPI
- No additional tools needed to start hybrid programs
  - `srun` **does all the miracle work**
    - or `mpirun` in Intel MPI – provided the environment is set up correctly
    - no need for `vsc-mympirun` (still used by some VSC sites)

Running a hybrid OpenMP/MPI job

generic-hybrid.slurm

```
#!/bin/bash

#SBATCH --job-name hybrid_hello
#SBATCH -A ap_course_hpc_intro
#SBATCH --ntasks=8 --cpus-per-task=16          ← 8 MPI processes with 16 threads
#SBATCH --partition=zen2 --nodes=2             ← make sure the job uses 2 Vaughan compute
                                                  nodes (to avoid cluttering)

module --force purge
module load calcua/2024a                       ← load the software stack module
module load vsc-tutorial/202203-intel-2024a    ← load vsc-tutorial – also load
                                                  the Intel toolchain
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK    ← set the number of (OpenMP) threads to use
export OMP_PROC_BIND=true                      ← threads stay on the core where they're created

srun -c $SLURM_CPUS_PER_TASK mpi_omp_hello     ← run the MPI program (mpi_omp_hello)
                                                  srun does all the magic
```

Job monitoring — Commands for interactive monitoring

- When your job is running
  - how do I know how much memory my job is using?
  - how can I check if my job is running properly, i.e. using the allocated CPUs?

- While your job is running, you can log on to the compute nodes assigned to that job
  - check which compute nodes a job uses: `squeue -j <jobid>`
  - log on to a compute node: `ssh <compute-node>`
  - run a command on all allocated nodes: `srun --jobid <jobid> --overlap <command>`

- When logged in on the compute node, check the behavior
  - **`htop`** → core & memory usage
  - **`sar`** → system performance metrics like CPU / memory / disk usage *over time*
  - **`vmstat`** → monitors system memory / processes / CPU activity / I/O statistics *in real-time*
  - **`pstree`** → display a tree view of the running processes

Job monitoring — The `monitor` module

- Add monitoring in your job script
  - sample a programs' metrics – CPU usage and memory consumption
  - can also check the sizes of (temporary) files
  - only single node jobs are supported — not MPI support
- Usage examples:
  - `monitor -d 30 -n 20 -l monitor.log <command>`
    - use a sample rate (delta) of 30 seconds, keep only the last 20 results, and log to a file
  - `monitor -f file1.tmp,file2.tmp <command>`
    - check the size of the (temporary) files
  - `monitor -d 60 -- matlab -nojvm -nodisplay computation.m`
    - delimit the monitor's options (to avoid confusion)

Monitoring memory and CPU usage of programs

Github repository for monitor — by Geert Jan Bex

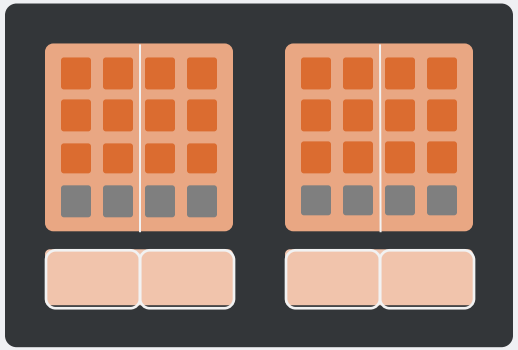
Hands-on

- Submit the parallel jobs from this section using the provided job scripts
  - a shared memory (OpenMP) job: `prime-omp.slurm`
  - a distributed memory (MPI) job: `prime-mpi.slurm`
  - a hybrid OpenMP/MPI job: `prime-hybrid.slurm`

- While the jobs are running
  - check where the job is running
  - log on to the first node allocated to that job
  - run the job monitoring commands
    - is your job behaving properly?

- When your job finishes
  - check the output files

Summary — Multi-core parallel jobs



- The key to supercomputing is **parallelization**
- A program can be parallelized in 2 ways:
  - **shared memory**: multithreading
  - **distributed memory**: multiprocessing (needs a program starter like `srun`)
- You should monitor your computation to ensure resources are used properly

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8 — Multi-job submission

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Running a large batch of small jobs

- Scenario: you want to run many, many, many small (short/serial) jobs
  - but: submitting and tracking many short jobs → *burden on scheduler*
- Solutions:
  - **Job arrays**: submit a large number of related yet independent jobs at once
    - to manage array jobs, use `atools`
  - **srun** can be used to launch more tasks than requested in the job request
    - running no more than the indicated number of tasks simultaneously
  - GNU **parallel**: tool to easily run shell commands in parallel with different inputs
    - general-purpose tool, can be used in multiple scenarios
- Note: these independent (sub) jobs can also run simultaneously across multiple nodes

Job arrays

- Starts from a job script for a single (sub) job in the array

job_array.slurm

```
#!/bin/bash
#SBATCH --ntasks=1 --cpus-per-task=1
#SBATCH --mem-per-cpu=512M
#SBATCH --time 15:00

INPUT_FILE="input_${SLURM_ARRAY_TASK_ID}.dat"
OUTPUT_FILE="output_${SLURM_ARRAY_TASK_ID}.dat"

./calculation ${SLURM_ARRAY_TASK_ID} -input ${INPUT_FILE} -output ${OUTPUT_FILE}
```

← for every run, there is a separate input file and an associated output file

- Specify the number of (sub) jobs in the array

```
sbatch --array 1-100 job_array.slurm
```

- Result: the program will be run for all input files (100)

Job arrays – atools

- Features of **atools**
  - provides a logging facility and commands to investigate the logs
    - which items failed or did not complete → restart only those
  - has limited support for Map-Reduce scenarios
    - preparation phase → split up data in manageable chunks
    - process all chunks in parallel
    - postprocessing phase → combine the results into one file
- `atools` versus `GNU parallel`
  - `atools` uses job arrays: relies on the scheduler to start all work items
  - while `parallel` starts the work items itself, but cannot start work items on another node

atools – by Geert Jan Bex

atools example – Parameter exploration

- The **field names** of the header in the CSV file are used as **variables** inside the job script

weather.slurm

```
#!/bin/bash
#SBATCH --ntasks=1 --cpus-per-task=1
#SBATCH --time=10:00
module --force purge
module load calcua/2024a atools/1.5.1

source <(aenv --data data.csv)
./weather -t $temperature -p $pressure -v $volume
```

data.csv

```
temperature, pressure, volume
293.0,       1.0e05,   87
...,         ...,      ...
313,         1.0e05,   75
```

input data in **CSV** format

- Run weather for all data values (from data.csv)

```
module load atools/1.5.1
sbatch --array $(arange --data data.csv) weather.slurm
```

Summary — Multi-job submission

- Another type of parallelization is *embarrassingly parallel* (or **high throughput**), where all the tasks are independent
- Slurm supports **job arrays** to submit a job script multiple times
- `atools` helps you manage job arrays
  - get parameters from a .csv file
  - rerun failed jobs
  - combine/aggregate data

Hands-on

- *Round the table questions*
  - *what type of software will you be running?*
  - *which scenario applies most to your use case?*
    - will you be running large parallel jobs — make sure your jobs use all the resources
    - or some medium-sized jobs
    - or lots of small jobs — try bundling the jobs whenever possible
  - *how will you be organizing your jobs?*
    - will (most of) your jobs use a similar job script — try using variables and arguments
    - will your jobs depend on each other or are they independent
- Discuss with your neighbours and check out the (relevant) extra examples in `more_examples`

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9 — Installing your own software

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Installing your own software

- Custom software should be installed in your own directory — *preferably in* `$VSC_DATA`
- If the package is supported by **EasyBuild**
  - modify an existing build script — *called "easyconfig"*
  - use our helper script to setup an EasyBuild environment (under `$VSC_DATA/easybuild`)

```
source init-easybuild-user.sh
```

- Otherwise: **manually install** the package
  - find the building instructions for the package
  - load a (sub)toolchain module and other modules that provide the libraries you need
  - make sure to set the proper options for the architecture
- Alternative: use **Apptainer containers** instead → *see next slides*

EasyBuild documentation and tutorial

Installing your own packages

- Python (`pip`), R, Julia, ... packages
  - load an appropriate Python, R, Julia, ... module
  - point the install prefix to an appropriate directory
    - e.g.: `R_LIBS_USER`, `JULIA_DEPOT_PATH` → in a subdirectory of `$VSC_DATA`
  - note: when using `pip`, also change the location of the cache directory `~/.cache` → *file quota!*

- Conda environments are *discouraged*
  - installations involve many small files → *file quota!*
  - typically, they do not use system and software stack libraries – possible performance issues
  - consume a lot of disk space and put stress on the filesystem
  - **alternative** → *wrap the Conda environment in a container*

Installing packages using `pip`

R package management

Using containers – hpc-container-wrapper

- Solution: use **hpc-container-wrapper** – *formerly known as Tykky*
  - tool to wrap your Python installation into a container, designed for use on HPC systems
  - uses `environment.yaml` (Conda) or `requirements.txt` (pip) to build a container image
  - provides wrapper scripts to transparently call executables within the container environment
    - also provides **wrap-container** to generate wrapper scripts for an existing container

- Create the container with **conda-containerize**

```
$ module load hpc-container-wrapper
$ conda-containerize new --prefix
  "$VSC_SCRATCH/bsoup" environment.yaml
```

- Similar for **pip-containerize**

environment.yaml

```
name: bsoup4
channels:
  - conda-forge
dependencies:
  - beautifulsoup4
  - ...
```

Using containers – hpc-container-wrapper

- Use your containerized Python installation (e.g., from within a job)

```
$ export PATH="$VSC_SCRATCH/bsoup/bin:$PATH"
$ which python
$VSC_SCRATCH/bsoup/bin/python
$ python -c "from bs4 import BeautifulSoup; soup = BeautifulSoup('<p>Hello World</p>', 'html.parser'); print(soup.p.text)”
Hello World
```

- Still missing packages? → update the container

```
$ conda-containerize update --post-install
  post.sh "$VSC_SCRATCH/bsoup"
```

post.sh

```
pip install requests
conda install -c bioconda pyfaidx
```

Github repository or documentation

Using containers – apptainer

- **Apptainer** is available to build and run your container images
  - *note: Docker is typically not supported due to security concerns*
- Option: convert a (pre-build) Docker *image* to Apptainer

```
$ apptainer pull docker://hello-world:latest
$ apptainer run hello-world_latest.sif
```

- Alternative: build an image from scratch using build scripts
  - called *definition files* – similar to a Dockerfile

```
$ export APPTAINER_CACHEDIR=$VSC_SCRATCH/apptainer/cache
$ export APPTAINER_TMPDIR=$(mktemp -d -p /dev/shm)
$ apptainer build ubuntu_fpc.sif ubuntu_fpc.def
$ apptainer exec ubuntu_fpc.sif fpc -h
```

ubuntu_fpc.def

```
BootStrap: docker
From: ubuntu:oracular

%post
    apt-get update
    apt-get install -y fpc
```

- Can I run containers on the HPC systems?
- Containers for HPC — VSC course, with GitHub repository — by Geert Jan Bex

Summary — Installing your own software

- You can install your own software, using:
  - Easybuild
  - manual install
  - Apptainer
- Sometimes **Conda environments** are necessary
  - `hpc-container-wrapper` is strongly recommended

HPC@UAntwerp introduction

10 — Interactive applications

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Running interactive applications on the compute nodes

- With `sbatch` you run jobs on compute nodes *without user interaction*
  - you need to provide all the input in advance
  - you cannot interact with the script or program while it is running

- Sometimes, you need to interact with a running program
  - when building software on a compute node in an interactive shell
  - when running an interactive Python session in a Jupyter notebook
  - when developing software using a dedicated IDE (integrated development environment)

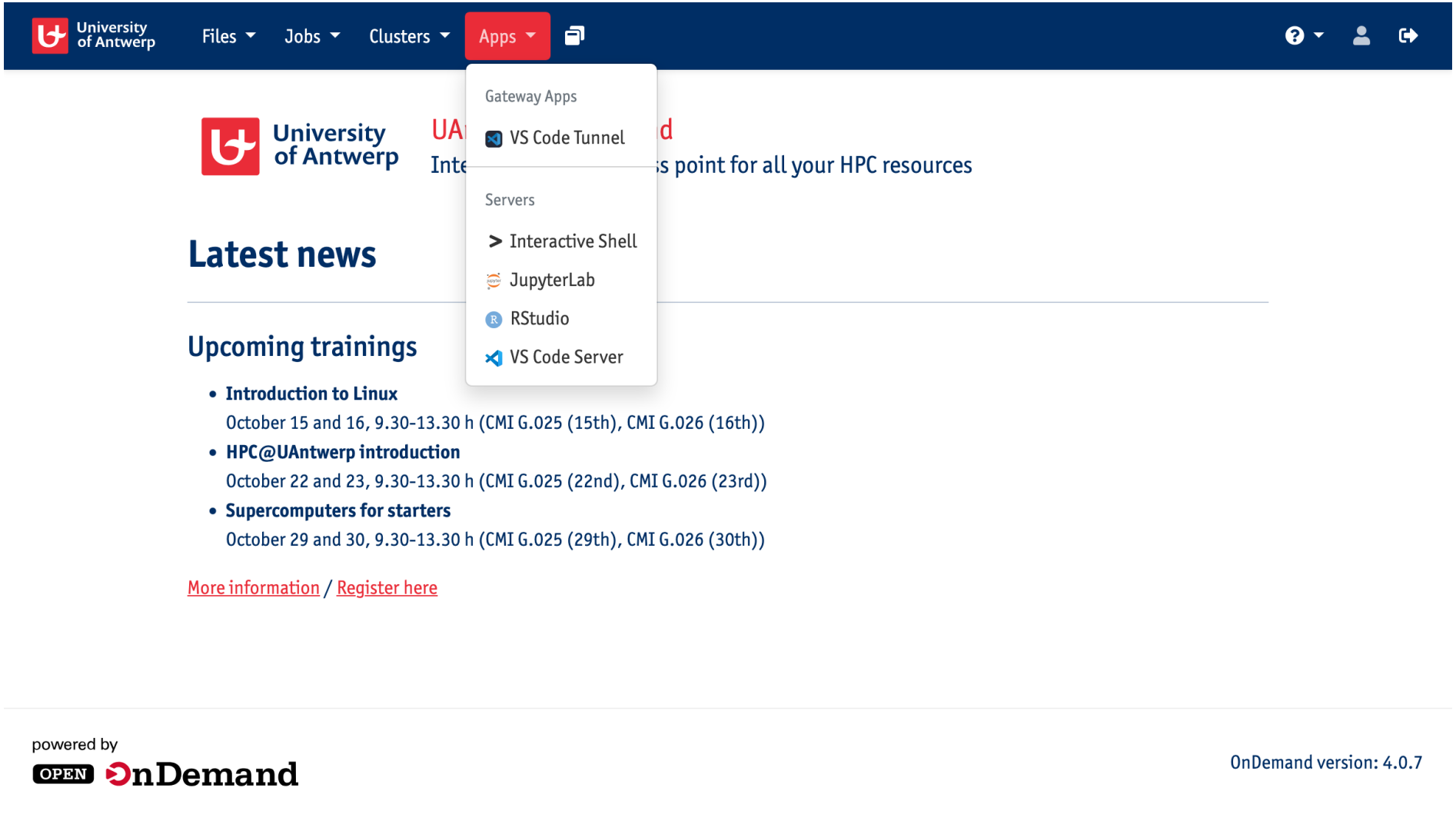
- You can run interactive applications on the compute nodes
  - using web portal apps
  - with `srun --pty bash`
  - or using `ssh`

Web portal apps — New

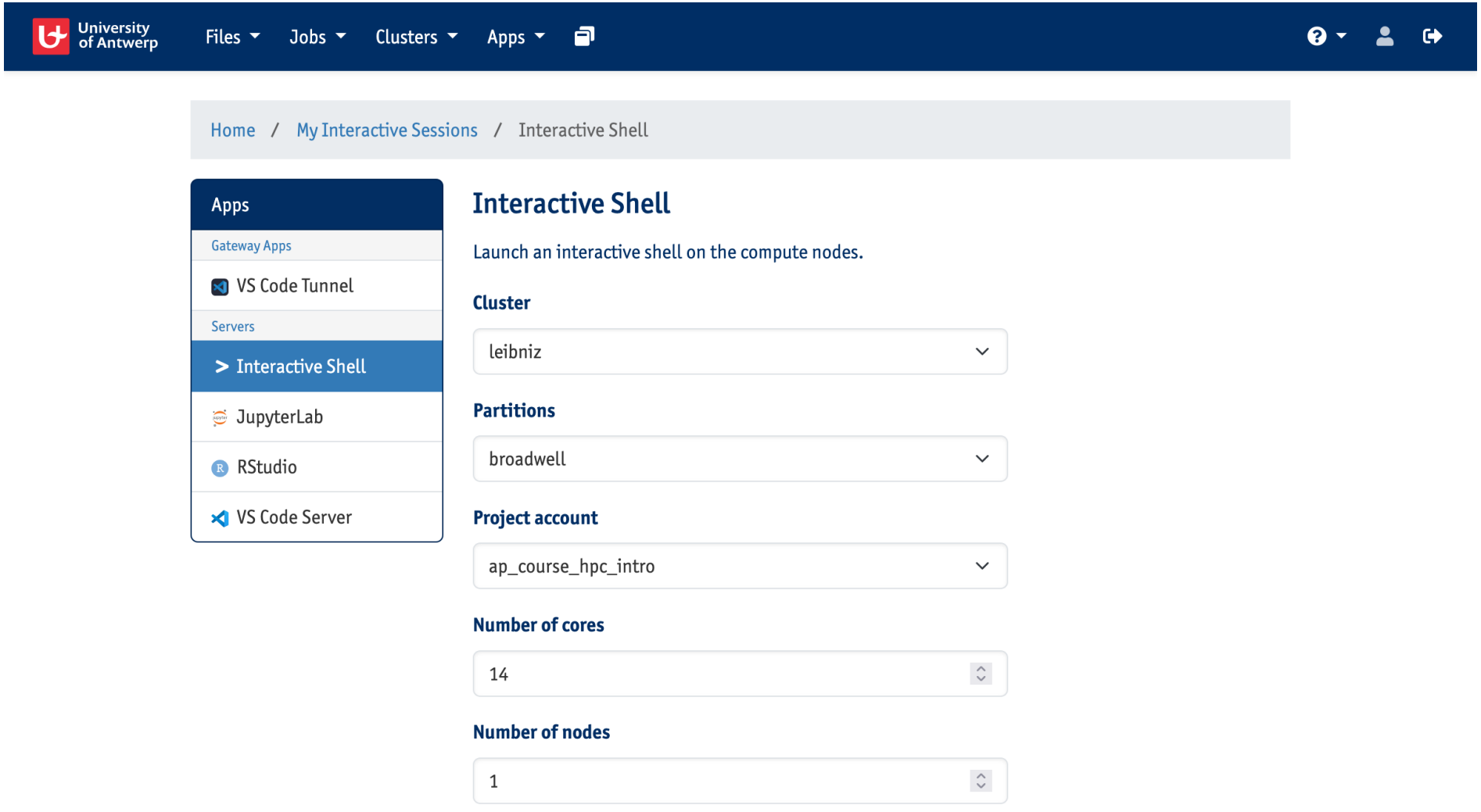
- Currently available — *more apps will be added*
  - Interactive Shell
  - JupyterLab
  - RStudio Server
  - VS Code Server or VS Code Tunnel
    - *I have VS Code installed on my pc* → VS Code Tunnel suggested
- *Important: interactive apps keep on running if you close the browser window*
  - *you need to explicitly cancel the app listed in "My Interactive Sessions"*

Open OnDemand — apps listed in navigation panel on the left

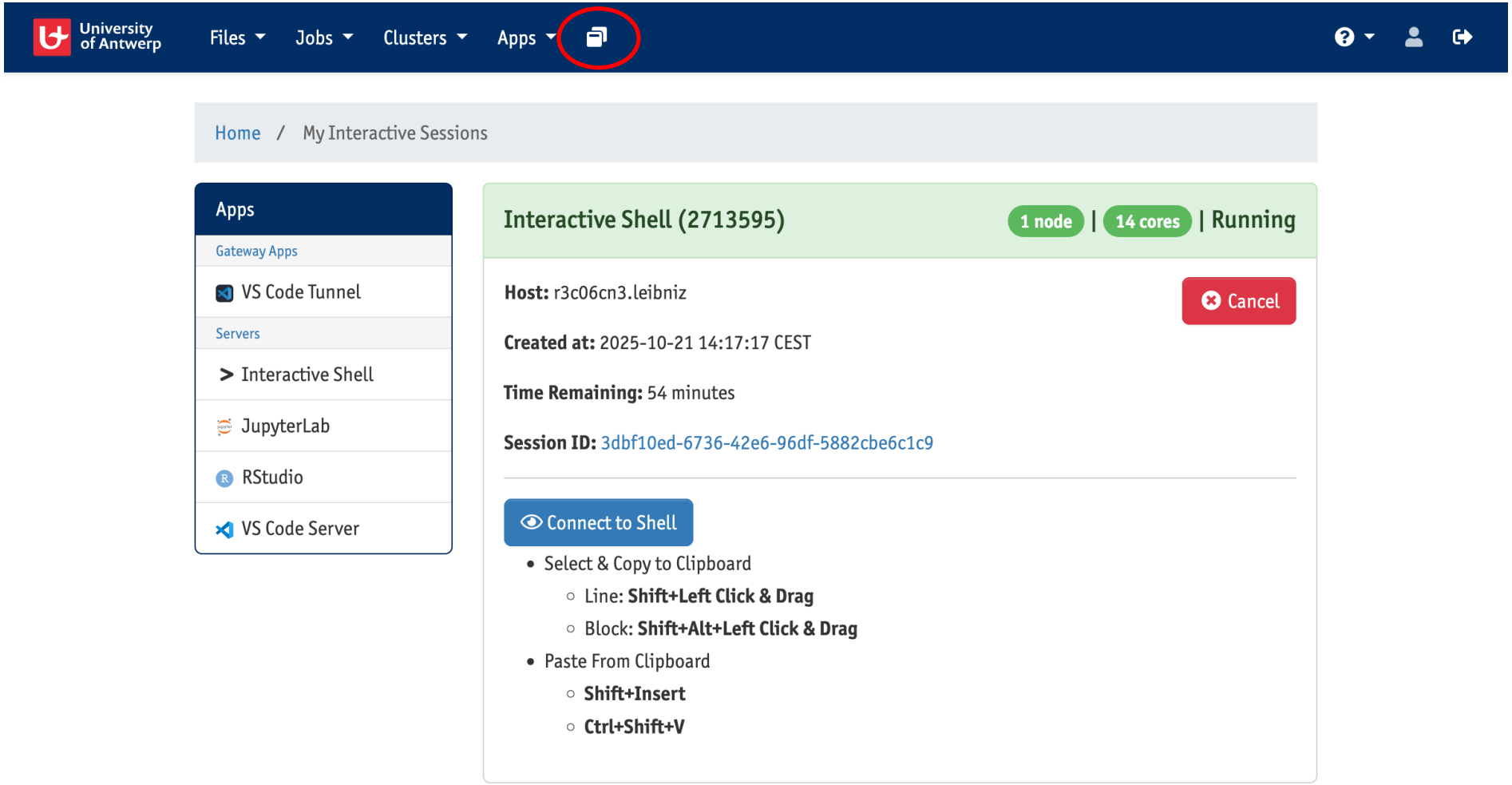
Web portal apps — New



Web portal apps — Interactive Shell

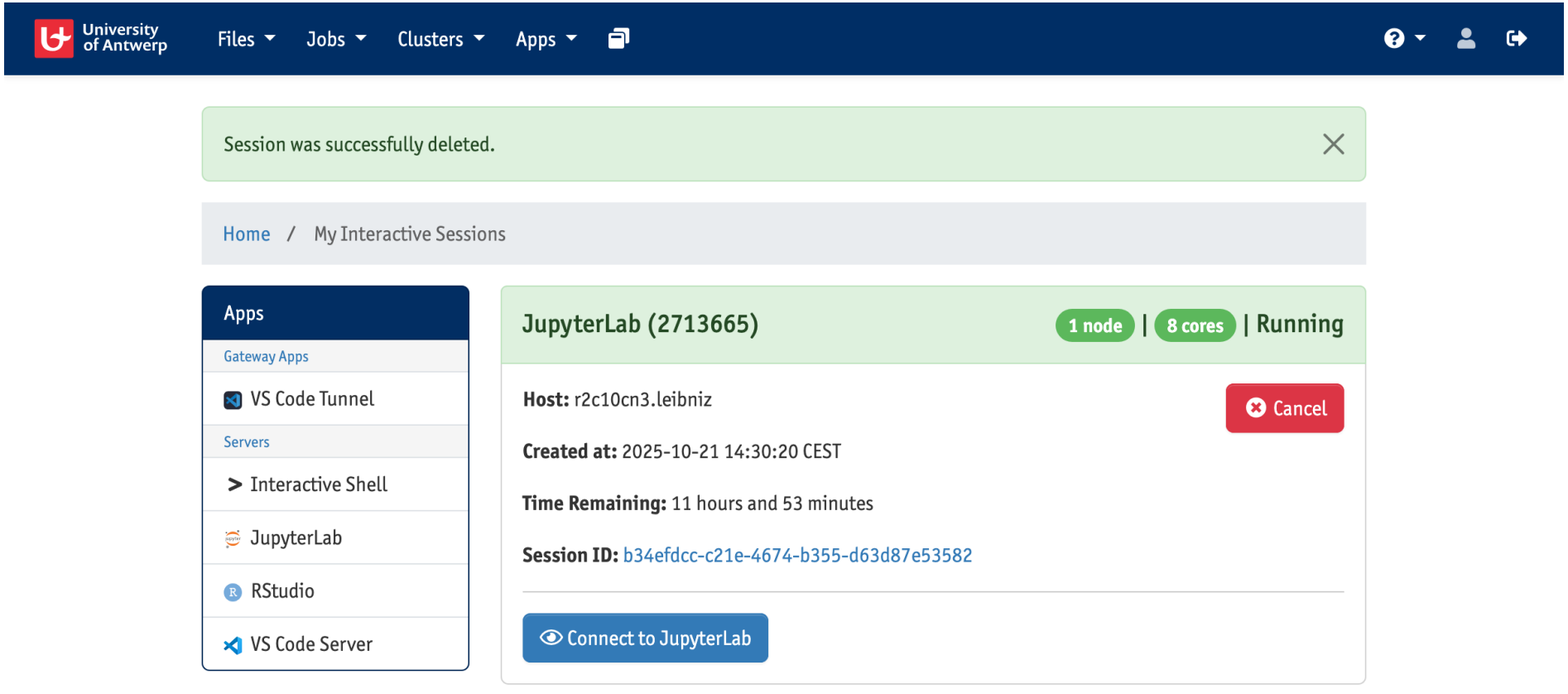


Web portal apps — Interactive Shell

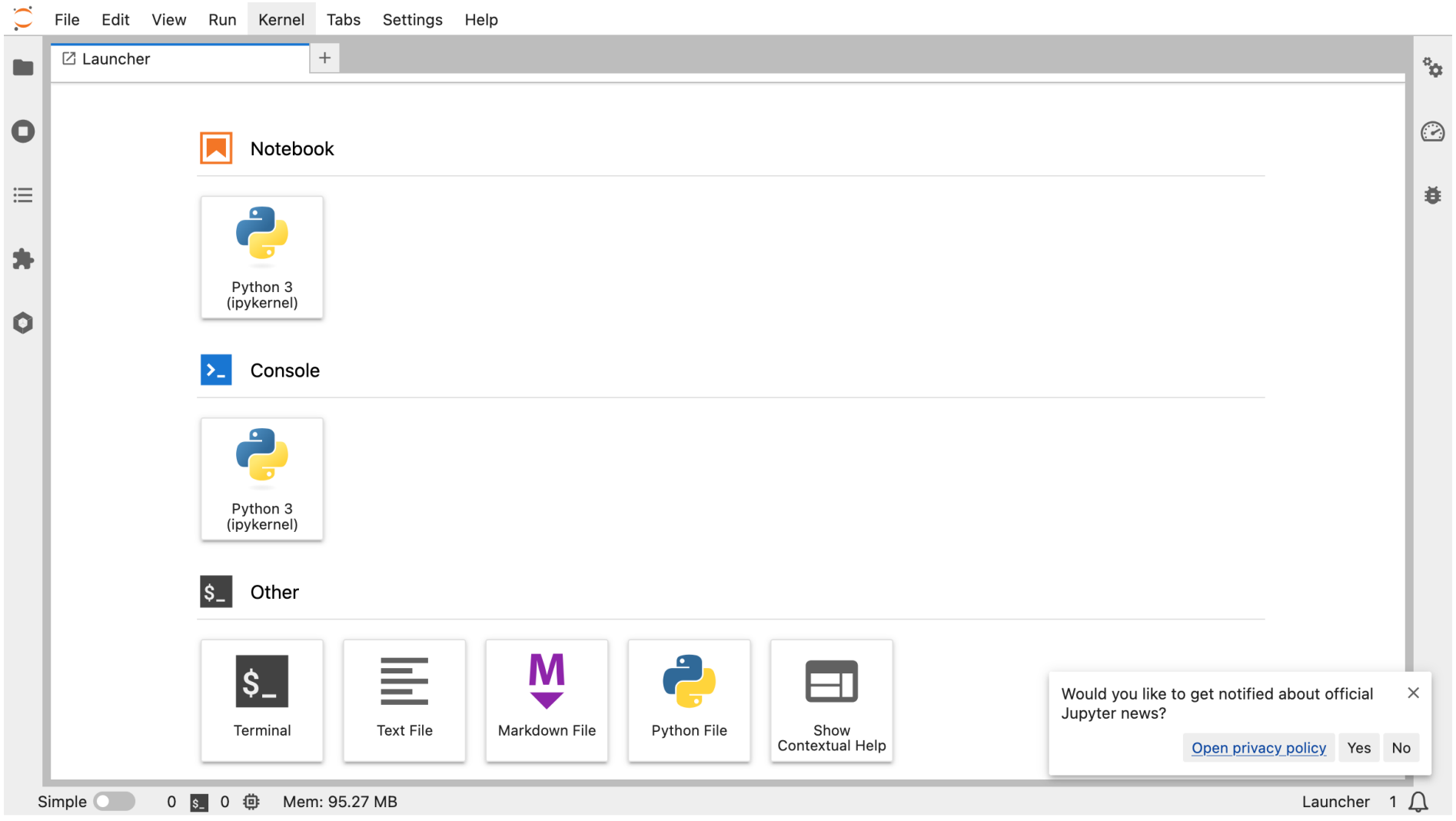


Web portal apps — Interactive Shell

Web portal apps — JupyterLab



Web portal apps — JupyterLab



Using the visualisation node

- *Note: will soon be replaced by a desktop portal web app*

- Use case: sometimes running GUI programs is necessary – e.g.: for visualisation of results
  - and some GUI programs need GPU-accelerated hardware — e.g., `GaussView`, `MonolixSuite`

- Leibniz has one *visualisation node*: **viz1.leibniz**
  - NVIDIA Quadro Pascal P5000 GPU
  - has Xfce as desktop/window manager
  - uses VirtualGL for graphics acceleration → e.g.: `vglrun glxgears`

- To access to remote desktop, you need to
  - use a **VNC** client, such as TurboVNC or TigerVNC
  - setup an SSH-tunnel (when accessing from outside Belgium)

Remote visualisation @ UAntwerp

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X — Extra topics

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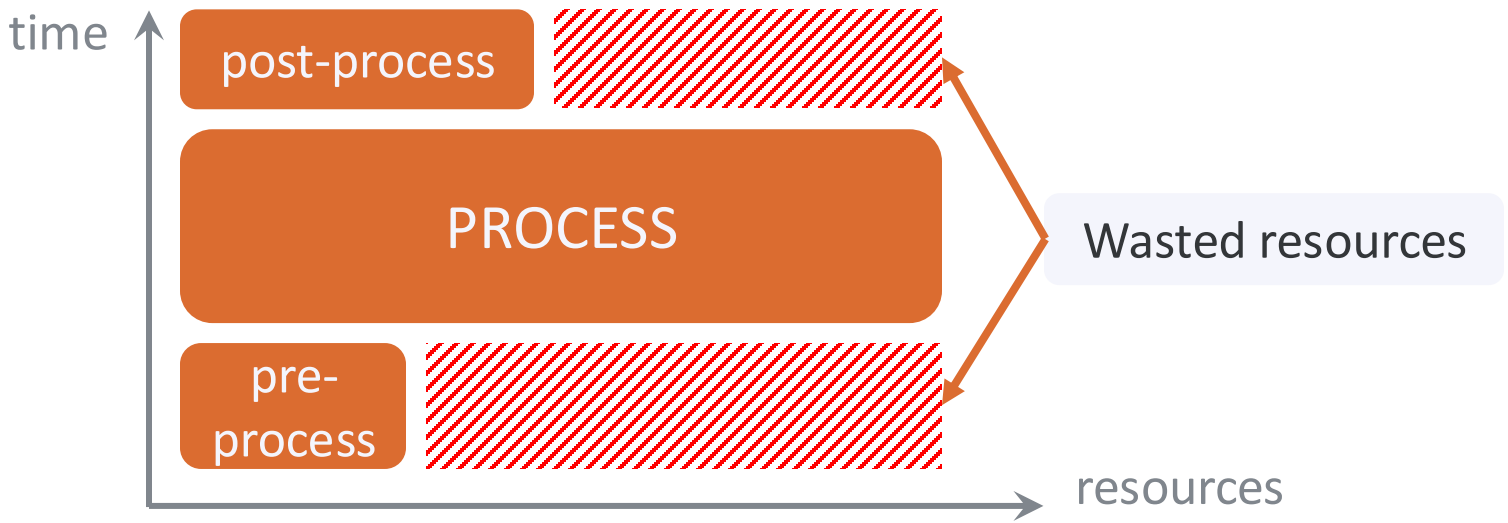
Job workflows — Examples

- Some scenarios
  - run simulations using results of a previous simulation, but with a different number of nodes
    - e.g., in CFD: first a coarse grid computation, then refining the solution on a finer grid
  - perform extensive sequential pre- or postprocessing of a parallel job



Job workflows — Examples

- Some scenarios
  - run simulations using results of a previous simulation, but with a different number of nodes
    - e.g., in CFD: first a coarse grid computation, then refining the solution on a finer grid
  - perform extensive sequential pre- or postprocessing of a parallel job
  - run a sequence of simulations, each depending on result of previous one
    - what to do when the max. wall time is reached?
  - run a simulation, apply perturbations to the solution
    - then run subsequent simulations for each perturbation
- Workflow = order in which the jobs will be submitted or run

Job workflows — Passing variables to job scripts

- Remember: on UAntwerp clusters, only a minimal environment is passed to the job
- Variables need to be passed *explicitly*, otherwise `sbatch` will not see them
  - propagate a value of (already existing) environment variables

    ```
    sbatch --export=<myenv1>,<myenv2>
    ```

  - pass a variable with given value to the job environment

    ```
    sbatch --export=<myenv>=<value>
    ```

  - *note:* `SLURM_*` *variables are always propagated*

Job workflows — Passing arguments to job scripts

- Command line arguments for the job script are passed *after the name of the job script*
  - Create a test script

get_parameter.slurm

```
#!/bin/bash
#SBATCH --ntasks=1 --cpus-per-task=1
#SBATCH --mem-per-cpu=500m
#SBATCH --time=5:00

echo "Hello $1."
```

  - Now run

```
sbatch get_parameter.slurm people
```

  - The output file will contain

```
Hello people.
```

Job workflows — Job dependencies

- You can instruct Slurm to start a job only
  - when some (or all) jobs from list of jobs have *ended*

    ```
    sbatch --dependency=afterok:<jobid>
    ```

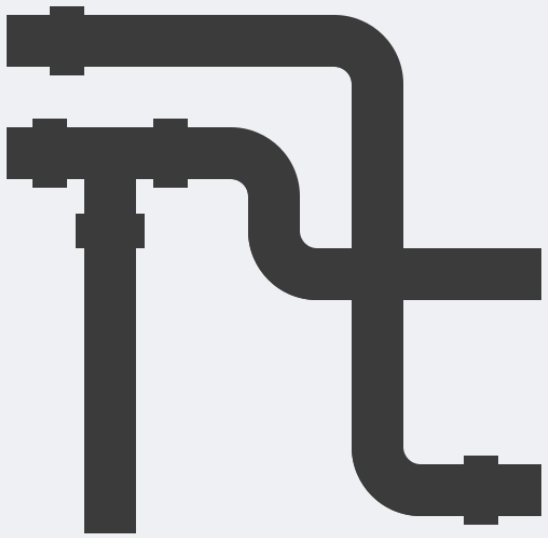
  - after a job has *failed*

    ```
    sbatch --dependency=afternotok:<jobid>
    ```

- Useful to organize series of (subsequent) jobs
  - powerful in combination with environment variables
  - or command line arguments passed to job scripts

the sbatch manual page – look for `--dependency`

Summary — Job workflows



- A **workflow** is the order and rules that decide how jobs run
- Slurm supports job **dependencies**, where a job can only start after another job has ended

  ```
  $ sbatch --dependency=...
  ```

- You can pass environment variables and arguments to a job

  ```
  $ sbatch --export=ENVVAR job.sh arg
  ```

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Final notes

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Some best practices

- Before starting to submit jobs, you should always check
  - are there any errors in the script?
  - are the required modules loaded?
  - is the correct executable used?
  - did you use the right process starter (srun)?
  - does the job start in the right directory?

- Check your jobs at runtime
  - login to a compute node and inspect your jobs
    - If you see that the CPU is idle most of the time that might be the problem
  - check the job accounting information (e..g.: MinCPU and AvgCPU)
  - alternatively: run an interactive job for the first run of a set of similar runs
  - try to benchmark the software for (I/O) scaling issues when using MPI

Warnings

- Avoid submitting many small jobs (in number of cores) by grouping them
  - using a job array
  - or using `atools`
- Runtime is limited by the maximum wall time of the partition
  - for longer wall time, use checkpointing
  - properly written applications have built-in checkpoint-and-restart options
- Requesting many processors could imply lon waiting times
  - though we're still trying to favour parallel jobs

what a cluster is not

a computer that will automatically run the code of your (PC) application much faster or for much bigger problems

Some site policies

- Our policies on the cluster
  - nodes are shared resources
  - priority based scheduling – so not “first come, first get”
  - fairshare mechanism – to make sure one user cannot monopolise the cluster
  - Accounting @ CalcUA → using a project account is mandatory

- Implicit user agreement
  - the cluster is valuable research equipment
  - *do not use it for other purposes than your research for the university*
    - no cryptocurrency mining or SETI@home and similar initiatives!
    - not for private use
  - you have to acknowledge the VSC in your publications

- Do not share your account nor your keys

Project accounts and credits

- At **UAntwerp Tier-2**, we use accounting — as of March 2024
  - using a project account is mandatory
  - billing is done for both computing (jobs) and storage (files)

- On **VSC Tier-1**, you get compute time allocation
  - number of core hours or GPU hours
  - enforced through project credits
  - requested through a *project proposal*
  - free test ride "Starting Grant" — motivation required

- On **KU Leuven Tier-2**, you need compute credits
  - bought directly via KU Leuven

Project access Tier-1

Credits to use KU Leuven infrastructure

User support

- **Questions?** → contact us via **hpc@uantwerpen.be**
  - offices @ **CMI — G.309-G.313**
- mailing-list for announcements: calcua-announce@lists.uantwerpen.be
  - every now and then a more formal “HPC newsletter”
- Some guidelines for help
  - be as precise as possible – e.g.: give job id, submit dir, output files, …
  - help us help you – read (and understand) the relevant documentation

CalcUA website – VSC docs – Slurm docs

The end

Course feedback

- Please fill in our short questionnaire before Nov 1st
- Let us know what you liked and how we can improve our courses
- *Thank you for your participation!*

More training

- HPC core facility CalcUA
  - Introduction to Linux
  - HPC@UAntwerp introduction
  - Supercomputers for starters
- VSC Trainings
  - trainings organized by other VSC sites and abroad (including LUMI, and EuroCC)
- **Training sessions by Geert Jan Bex**
- Getting scientific software installed
  - 03 Nov 2025, 09:00 – 17:00 CET
  - Belpaire Building, Brussels