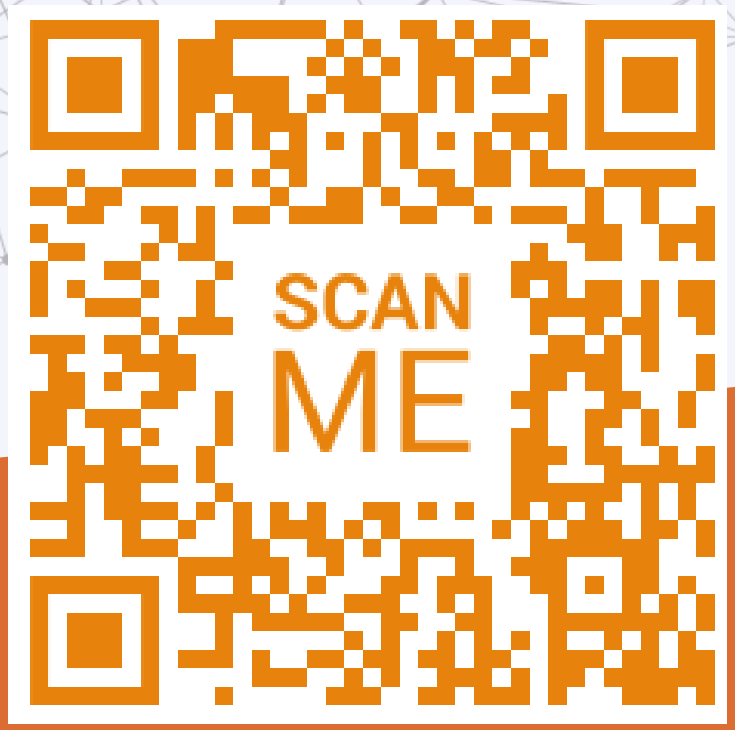
Vlaanderen
is supercomputing

Start with VSC

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



VLAAMS
SUPERCOMPUTER
CENTRUM

Innovative Computing
for A Smarter Flanders

vscentrum.be

Basics

- Request membership to lp_hpcinfo group (account.vscentrum.be)
- Login via OpenOnDemand: www.ondemand.hpc.kuleuven.be
  Features: File transfer, File editor, interactive apps, Jobs' overview
- Check disk quota:

```
$ myquota
```

- Check the credits

```
$ sam-balance
```

and

```
$ sam-list-allocations
```

- Software modules:

```
$ module {avail|list|load|unload|purge}
```

demo/test yourself

- Copy intro training files `/apps/leuven/training/HPC_intro/` to your `$VSC_DATA`
- Submit `cpujob` to the cluster
- List all your jobs `squeue -M wice`
- Check the information about the cpujob `slurm_jobinfo -M wice <job_ID>`
- Modify the `mpi.slurm` script to request 1 node, 72 cores for 30 minutes and get the notification about job start/end by e-mail
- Check the status of all the jobs

Command	Purpose
`$ sbatch ...`	Submit a batch job
`$ srun ...`	Submit an interactive job
`$ scancel --cluster=wice <JobID>`	Cancel a specific pending or running job
`$ scontrol show job --cluster=wice <JobID>` `$ slurm_jobinfo <JobID>`	Detailed job info (very useful to diagnose issues)
`$ squeue --cluster=wice --long`	Status of all recent jobs
`$ squeue --cluster=wice --start`	Give a rough estimate of start time
`$ sinfo --cluster=wice`	Info about the state of available partitions and nodes
`$ sacct --cluster=wice --batch --job <JobID>`	Show minimal info about a queue or partition (-p)
`$ slurmtop` `$ scontrol --cluster=wice show node <hostname>`	Overview of the cluster Get detailed information about the status of a node
`$ sam-balance`	Overview of all your available credit projects
`$ sam-list-allocations`	Detailed overview of your credit allocation history

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 resource usage (`htop`)

- Submit a batch GPU job
  - While the job is running get the information about the node `slurm_jobinfo...`
  - and check usage of resources on the node `ssh`, `top`, `nvidia-smi`

demo – conda installation

- Start an interactive job on Genius or wICE
  `srun –M genius –A <account> -n 1 --pty /bin/bash -l`
- Install miniconda in your `$VSC_DATA` directory

- `$ wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh`
- `$ DIR_INSTALL=$VSC_DATA/miniconda3_${VSC_INSTITUTE_CLUSTER}`
- `$ bash Miniconda3-latest-Linux-x86_64.sh -b –p ${DIR_INSTALL}`

- Add a PATH to conda:

- `$ export PATH="${VSC_DATA}/miniconda3_${VSC_INSTITUTE_CLUSTER}/bin:${PATH}"`

- Check if conda is added to your `$PATH ($ which conda)`

Add it to `$PATH` in your `.bashrc`

- `$ echo 'export PATH="${VSC_DATA}/miniconda3/bin:${PATH}" ' >> .bashrc`

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 – worker

- Copy intro training files (`/apps/leuven/training/worker/`) to your `$VSC_DATA`
- 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://docs.vscentrum.be/

VSC agenda: training sessions, events (VSC and KU Leuven user days)

Systems status page:
https://status.vscentrum.be

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