



Vlaanderen
is supercomputing

Start with VSC

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



VLAAMS
SUPERCOMPUTER
CENTRUM

*Innovative Computing
for A Smarter Flanders*

vscentrum.be

demo/test yourself

- ✓ Request membership to `lp_hpcinfo_training` group (Browse to www.account.vscentrum.be)
- ✓ Login with putty
- ✓ Filetransfer with Filezilla
- ✓ Login with NX
- ✓ Check disk quota
- ✓ Check the credits
- ✓ Restoring files from `.snapshot`
- ✓ Check/load/list/unload/purge module

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 (`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`)
- ✔ Submit an interactive job to GPU node
Run your program on a compute node
Open a new terminal and ssh to a compute node
Check the resources and GPU usage (`top`, `nvidia-smi` or `watch "nvidia-smi"`)
Submit a batch GPU job
- ✔ While the job is running get the information about the node (`checkjob`) and check usage of resources on the node (`ssh`, `top`, `nvidia-smi`)

demo – conda installation

✓ Install miniconda in your `$VSC_DATA` directory

- `$ wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh`
- `$ bash Miniconda3-latest-Linux-x86_64.sh -b -p $VSC_DATA/miniconda3`

✓ Add a PATH to conda:

- `$ export PATH="${VSC_DATA}/miniconda3/bin:${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 – 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_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

Systems status page:

<http://status.kuleuven.be/hpc>

*Stay Connected
to VSC*

Linked  [®]

