Vlaanderen
is supercomputing

VSC HPC demo session

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

VLAAMS
SUPERCOMPUTER
CENTRUM

Innovative Computing
for A Smarter Flanders

First steps

- Request to become a member of the *lp_hpcinfo* group via account.vscentrum.be
- Login via OpenOnDemand: ondemand.hpc.kuleuven.be
  Features: file transfer, file editor, interactive apps, job overview
- Check your disk quota:
  ```
  $ myquota
  ```
- Check your credit accounts:
  ```
  $ sam-balance
  $ sam-list-allocations
  ```
- Try the centrally installed software modules:
  ```
  $ module {avail|list|load|unload|purge}
  ```

First steps

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

Slurm command-line tools

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 --clusters=wice <JobID>` `$ slurm_jobinfo <JobID>`	Detailed job info (very useful to diagnose issues)
`$ squeue --clusters=wice --long`	Status of all recent jobs
`$ squeue --clusters=wice --start`	Give a rough estimate of when your jobs will start
`$ sinfo --clusters=wice`	Info about the state of available partitions and nodes
`$ sacct --clusters=wice --batch --job <JobID>`	Show the jobscript used for a given batch job
`$ slurmtop`	Overview of the cluster
`$ sam-balance`	Overview of all your available credit projects
`$ sam-list-allocations`	Detailed overview of your credit allocation history

Job monitoring

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

- Submit a GPU batch job
  - While the job is running, check its details with `slurm_jobinfo`
  - and check resource on the compute node using `ssh`, `htop` and `nvidia-smi`

Creating and using a Conda environment

- Start an interactive job on wICE
  ```
  $ srun -M wice -A <account> -n 1 --pty bash -l
  ```

- Go to your data folder
  ```
  $ cd ${VSC_DATA}
  ```

- Download Miniconda
  ```
  $ wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh
  ```

- Install Miniconda in your VSC_DATA
  ```
  $ bash Miniconda3-latest-Linux-x86_64.sh -b -p $VSC_DATA/miniconda3
  ```

- Permanently add the path to Miniconda to your `~/.bashrc`
  ```
  $ echo 'export PATH="${VSC_DATA}/miniconda3/bin:${PATH}" ' >> ~/.bashrc
  ```

Creating and using a Conda environment

- Create a Conda environment with some typical packages
  ```
  $ conda create -n science jupyter numpy scipy
  ```
- Activate this environment
  ```
  $ source activate science
  ```
- Verify that you can use what you installed
  ```
  $ python -c 'import scipy'
  ```
- Add one more package to this environment
  ```
  $ conda install matplotlib
  ```
- Return to your original environment
  ```
  $ conda deactivate
  ```

Useful links

Helpdesk (email): hpcinfo@kuleuven.be

Helpdesk (online form): https://admin.kuleuven.be/icts/HPCinfo_form/HPC-info-formulier

VSC website: https://www.vscentrum.be

VSC documentation: https://docs.vscentrum.be

VSC agenda, training sessions, events (User Day): https://www.vscentrum.be/vsctraining

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

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