CSC
Training for Brilliant Minds

Machine Learning at CSC

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Mats Sjöberg – mats.sjoberg@csc.fi

Overview

What CSC service to use?

Puhti supercomputer

Data storage

GPU utilization

Multi-GPU and multi-node jobs

Singularity containers

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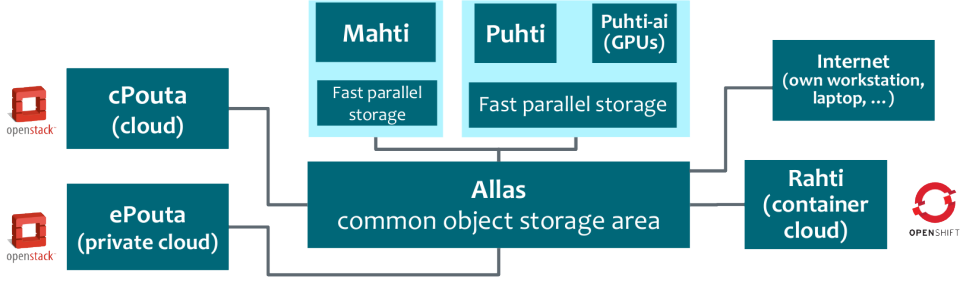
- CSC's supercomputer Puhti
- Virtual server on Pouta
- Container cloud Rahti



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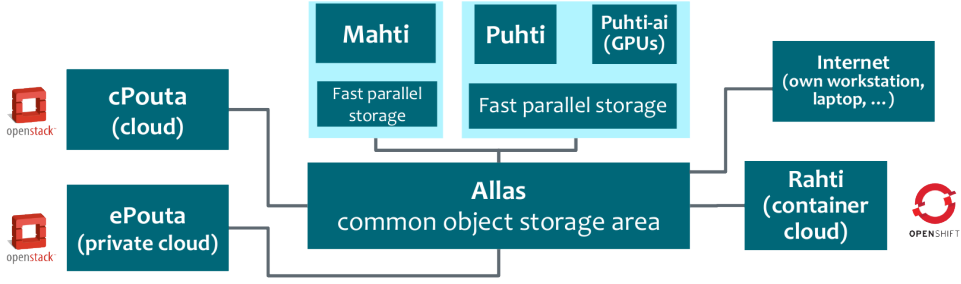

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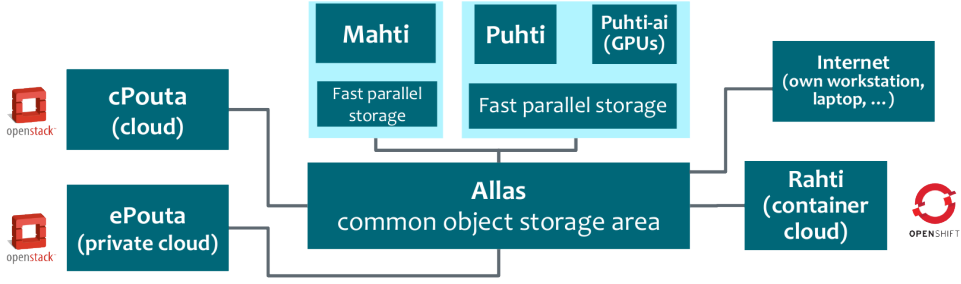

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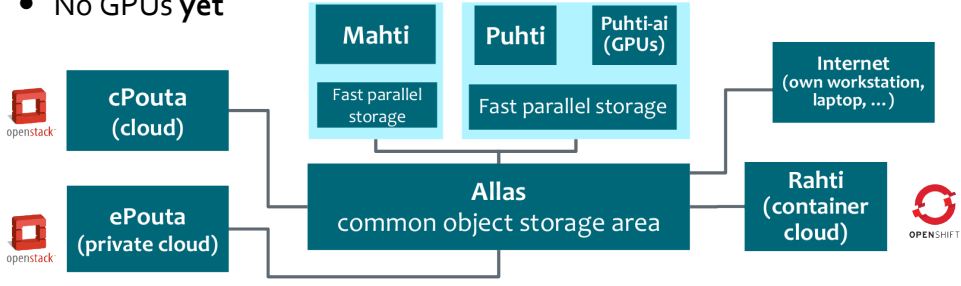
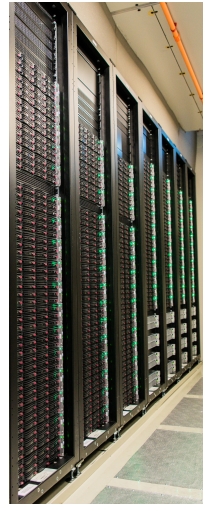
  - Easy to run containers
  - No GPUs **yet**



Puhti supercomputer

Puhti supercomputer

- *Puhti-AI*, cluster with 80 nodes with 4 GPUs each $\rightarrow$ 320 GPUs in total
- Latest generation Nvidia V100 GPUs (Volta) with 32 GB of memory
- Fast network: 2×100 Gbps links to each node
- Each node has a fast 3.2 TB local NVME disk



Getting access to Puhti

https://docs.csc.fi/computing/overview/

To use Puhti you need to:

- Have a CSC account
- Be member of a CSC project, either by
  - creating a new project, or
  - joining an existing project (ask the PI to add you!)
- Finally, the project needs to have Puhti access

→ MyCSC portal: https://my.csc.fi/

Accessing Puhti

- Using an ssh client such as OpenSSH or PuTTY
- Basic Linux skills are required!
- More info: https://docs.csc.fi/computing/connecting/

```
$ ssh <csc_username>@puhti.csc.fi
```

```
$ ssh <csc_username>@puhti-login2.csc.fi
```

Supported frameworks

We currently support:

- Python Data – collection of Python libraries for data analytics and machine learning
- TensorFlow – deep learning library for Python
- PyTorch – machine learning framework for Python
- MXNet – deep learning library for Python
- RAPIDS – suite of libraries for data analytics and machine learning on GPUs

`https://docs.csc.fi/apps/#data-analytics-and-machine-learning`

Example: TensorFlow

- First check the application page for instructions:
  https://docs.csc.fi/apps/tensorflow/
- Load the default version:
  `module load tensorflow`
- or specific version:
  `module load tensorflow/2.0.0`
- Note: some modules are *Singularity-based*!

What if some package is missing?

If you are using our module, but a trivial package is missing …

- install it yourself, e.g.,
  `pip install --user <packagename>`

- …or if it might be generally useful, send an email to `servicedesk@csc.fi` – we can install it for you!

What if some package is missing?

If you need a specific setup, and our modules are not right for you ...

- use a virtualenv:

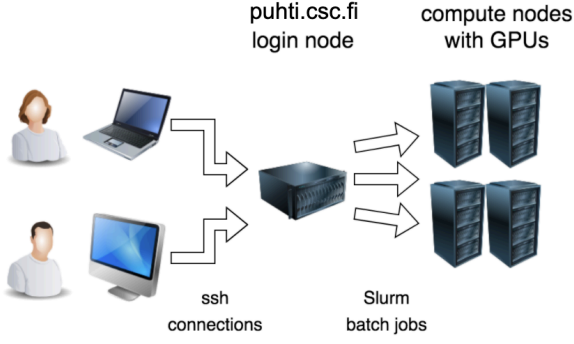
```
$ python3 -m venv myenv
$ source myenv/bin/activate
$ pip install ...
```

- use conda: https://docs.csc.fi/support/tutorials/conda/
- use singularity containers: https://docs.csc.fi/computing/containers/run-existing/
- or if generally useful, send an email to servicedesk@csc.fi

Running a job on Puhti

Don’t run heavy computing jobs in the login nodes!

- Puhti uses the *Slurm* batch job system
- Jobs do not run instantly but are put in a *queue*
- Resources (runtime, memory, number of cores) need to be specified



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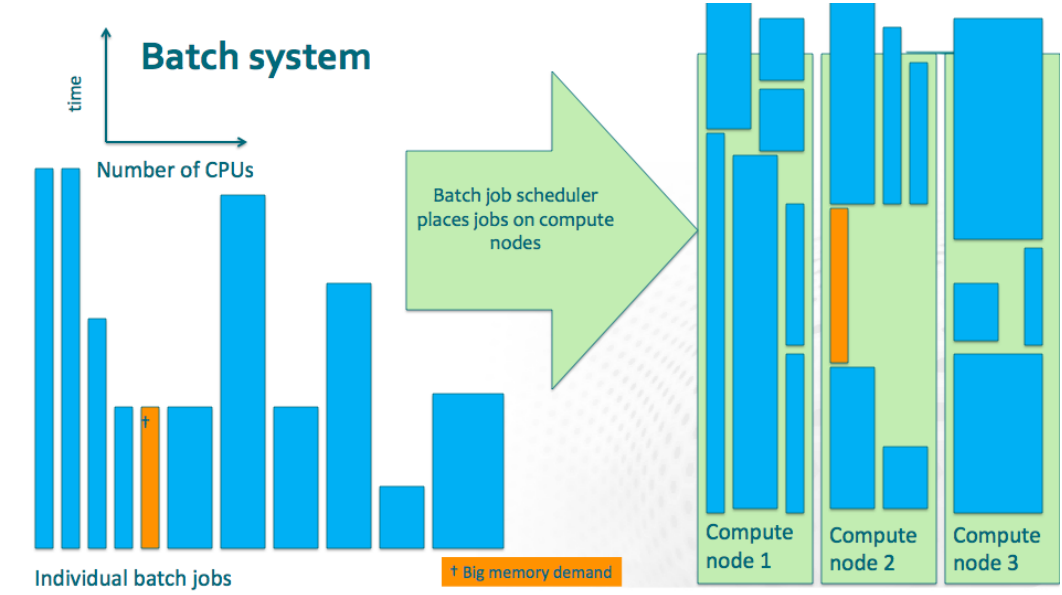

Running a job on Puhti

Create a job script, for example `run.sh`:

```
#!/bin/bash
#SBATCH --account=<project>
#SBATCH --partition=gpu
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=10
#SBATCH --mem=64G
#SBATCH --time=1:00:00
#SBATCH --gres=gpu:v100:1

module load tensorflow/2.0.0
srun python3 myprog.py <options>
```

https://docs.csc.fi/computing/running/creating-job-scripts/

Running a job on Puhti

Submit the job:

```
sbatch run.sh
```

Check the queue:

```
squeue -l -u $USER
```

Cancel a job:

```
scancel <jobid>
```

https://docs.csc.fi/computing/running/submitting-jobs/

Data storage

Data storage on Puhti

- Disk space and *number of files* are limited on Puhti!
  → We want to ensure that the shared (Lustre) filesystem works efficiently for everyone!
- Useful command: `csc-workspaces`

	Owner	Path	Capacity	Number of files	Cleaning
home	Personal	`/users/<user-name>`	10 GiB	100 000 files	No
projappl	Project	`/projappl/<project>`	50 GiB	100 000 files	No
scratch	Project	`/scratch/<project>`	1 TiB	1 000 000 files	Yes - 90 days

Data quotas can be increased via MyCSC!

https://docs.csc.fi/computing/disk/

Using Allas

- store big datasets in Allas, CSC's object storage
- download them to project scratch prior to computation
- you can also upload trained models (or keep in projappl)

```
$ module load allas
$ allas-conf
$ cd /scratch/<your-project>
$ swift download <bucket-name> your-dataset.tar
```

Large number of files

- Many datasets contain a large number of small files
- Shared filesystem (Lustre) performs poorly in this scenario
  $\rightarrow$ noticable slowdowns for all Puhti users!

Consider alternatives:

- packaging your dataset into larger files
- use NVME fast local storage on GPU nodes

Using more efficient data formats

Instead of many small files, use one or a few bigger files.

Examples:

- TensorFlow's TFRecord format
- HDF5
- LMDB
- ZIP, for example via Python's `zipfile` library

Fast local NVME drive

- All GPU nodes have a local NVME drive
- Just add `nvme:<number-of-GB>` to sbatch `--gres` flag

```
#!/bin/bash
#SBATCH --account=<project>
#SBATCH --partition=gpu
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=10
#SBATCH --mem=64G
#SBATCH --time=1:00:00
#SBATCH --gres=gpu:v100:1,nvme:100

tar xf /scratch/<your-project>/your-dataset.tar -C $LOCAL_SCRATCH

srun python3 myprog.py --data_dir=$LOCAL_SCRATCH <options>
```

GPU utilization

Multi-GPU and multi-node jobs

Singularity containers