



Training for Brilliant Minds

Machine Learning on Puhti

Part 1: Getting started

June 3, 2020

Mats Sjöberg – mats.sjoberg@csc.fi



Overview

What CSC service to use?

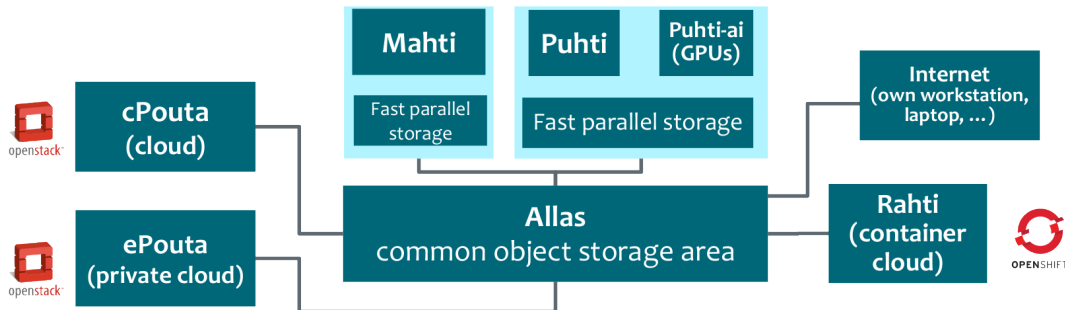
Getting access to Puhti

Running jobs on Puhti

Data storage

What CSC service to use?

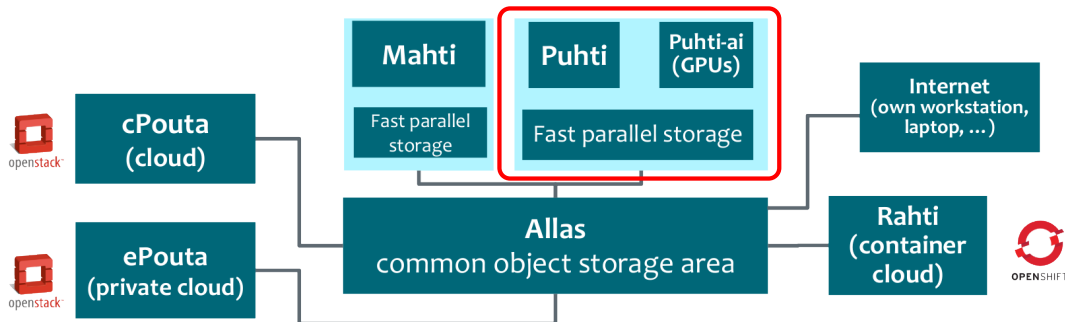
What CSC service to use?



What CSC service to use?

Puhti

- Supercomputer cluster
- GPU-accelerated nodes
- Multi-user system



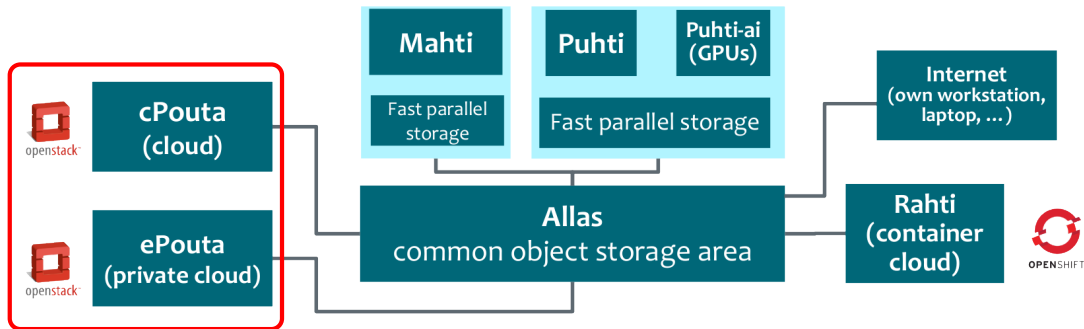
What CSC service to use?

Pouta

- Your “own” (virtual) server
- Less powerful than Puhti

Puhti

- Supercomputer cluster
- GPU-accelerated nodes
- Multi-user system



What CSC service to use?

Pouta

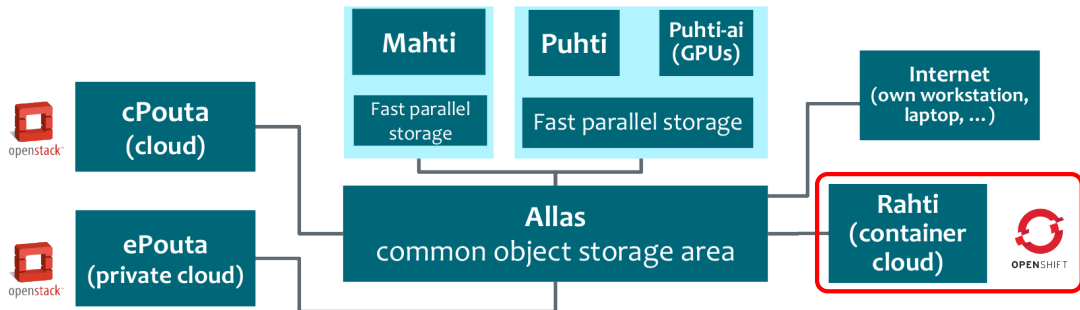
- Your “own” (virtual) server
- Less powerful than Puhti

Puhti

- Supercomputer cluster
- GPU-accelerated nodes
- Multi-user system

Rahti

- Container cloud
- No GPUs yet



What CSC service to use?

Pouta

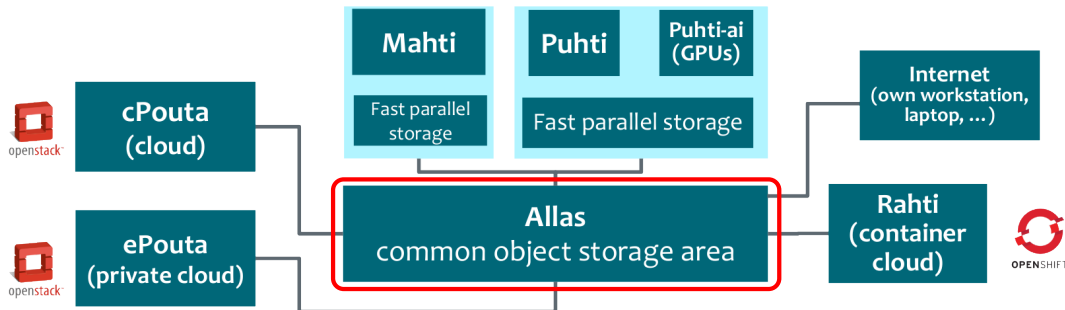
- Your “own” (virtual) server
- Less powerful than Puhti

Puhti

- Supercomputer cluster
- GPU-accelerated nodes
- Multi-user system

Rahti

- Container cloud
- No GPUs yet



What CSC service to use?

Pouta

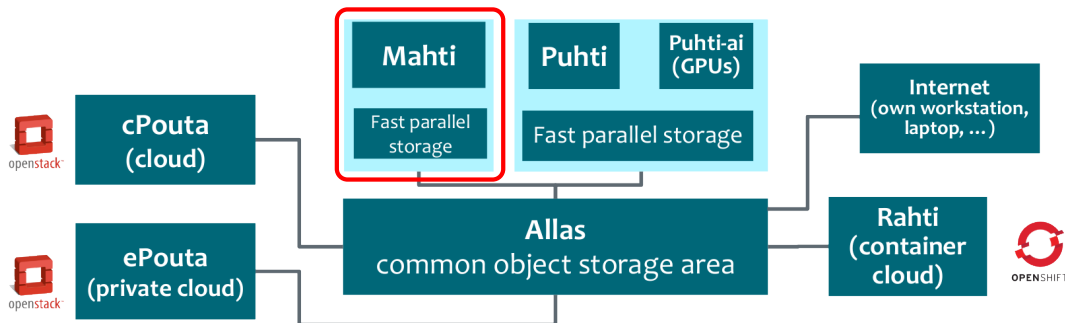
- Your “own” (virtual) server
- Less powerful than Puhti

Puhti

- Supercomputer cluster
- GPU-accelerated nodes
- Multi-user system

Rahti

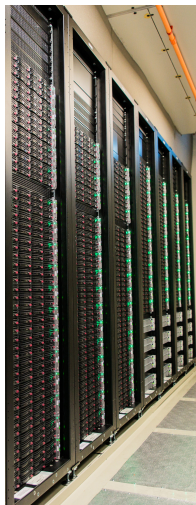
- Container cloud
- No GPUs yet



Getting access to Puhti

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
```

Running jobs on Puhti

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:

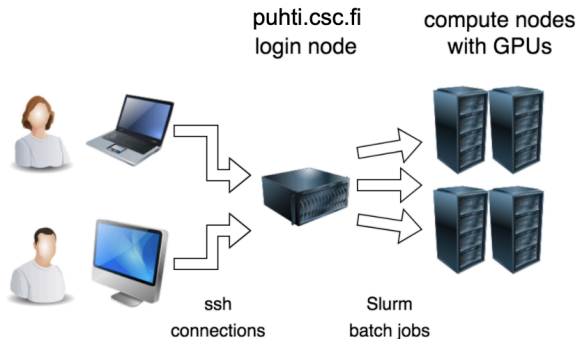
```
$ python3 -m venv myenv  
$ source myenv/bin/activate  
$ pip install ...
```

- 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

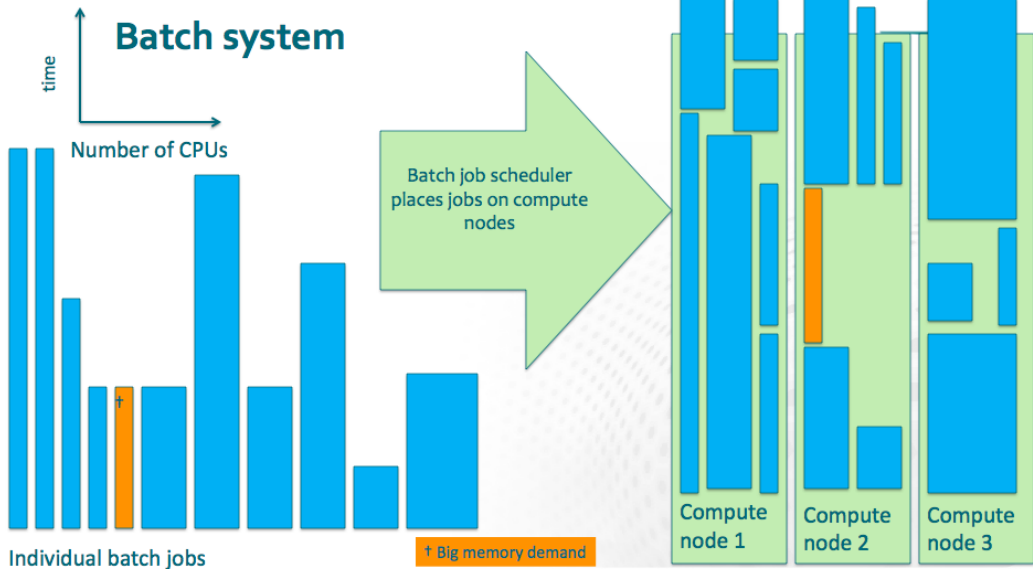
Running a job on Puhti

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



Running a job on Puhti



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

Example job script for Singularity-based modules:

```
#!/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/nvidia-20.03-tf2-py3
```

```
srun singularity_wrapper exec python3 myprog.py <options>
```

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
→ 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>
```

Thank you!

Don't forget part 2 of this webinar!

Machine Learning on Puhti

Part 2: Scaling up and using resources efficiently

- GPU utilization
- Multi-GPU and multi-node jobs
- Singularity containers

Time: Wednesday, June 10, 2020 at 14:00-15:00

Place: <https://ssl.eventilla.com/event/jJRkz>