CSC

Training for Brilliant Minds

Machine Learning at CSC

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Overview

What CSC service to use?

Puhti supercomputer

Data storage

GPU utilization

Multi-GPU and multi-node jobs

Singularity containers

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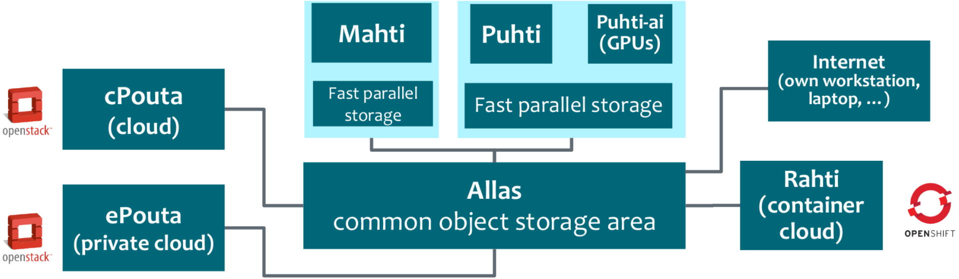
- CSC's supercomputer Puhti
- Virtual server on Pouta
- Container cloud Rahti



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  - Cluster with GPU-accelerated nodes
  - Multi-user environment
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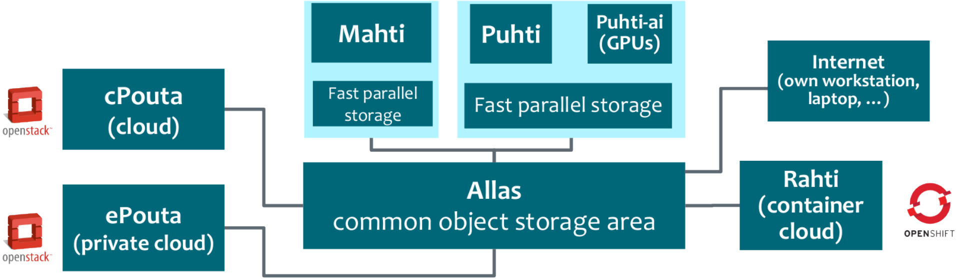
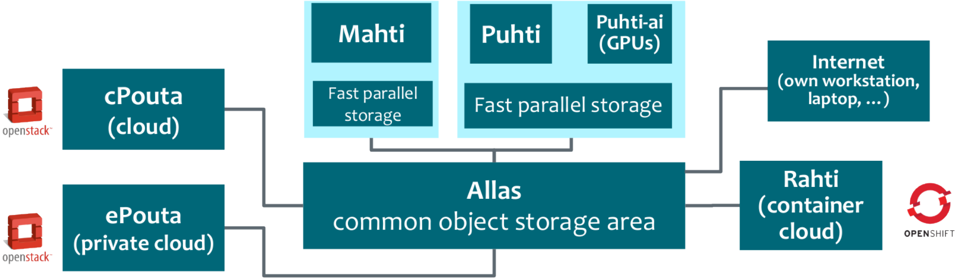


What CSC service to use?

- CSC's supercomputer Puhti
  - Cluster with GPU-accelerated nodes
  - Multi-user environment
- Virtual server on Pouta
  - Your "own" server
  - Less powerful than Puhti
- Container cloud Rahti



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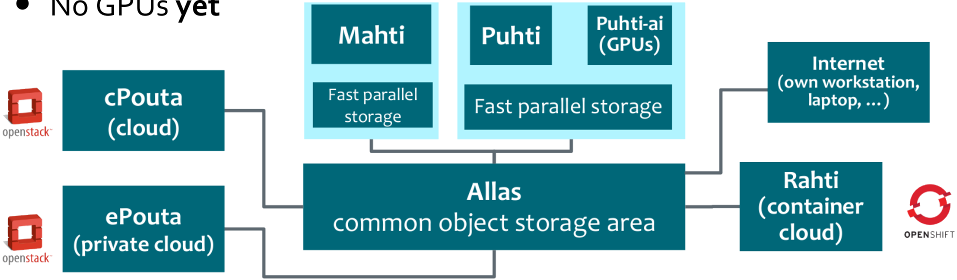
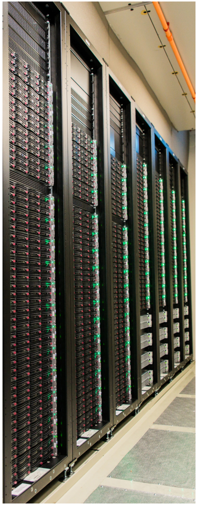
  - Less powerful than Puhti
- Container cloud Rahti
  - Easy to run containers
  - No GPUs **yet**



Puhti supercomputer

Puhti supercomputer

- *Puhti-AI*, cluster with 80 nodes with 4 GPUs each → 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:

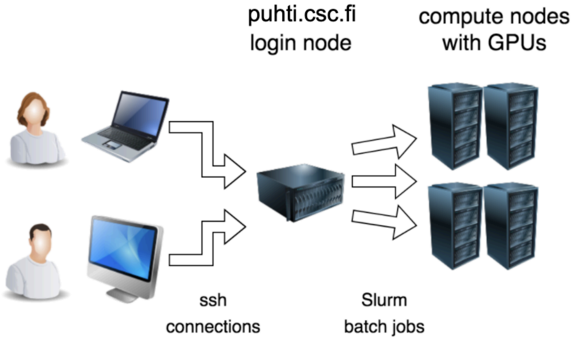
```
$ python3 -m venv myenv
$ source myenv/bin/activate
$ pip install ...
```

- 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

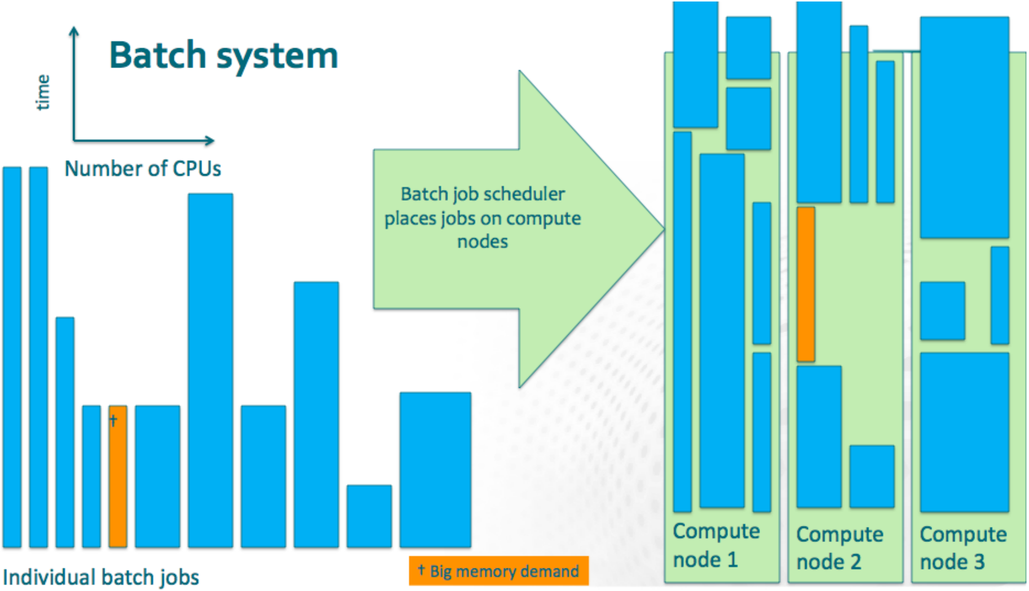
Running a job on Puhti

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



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

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>
```

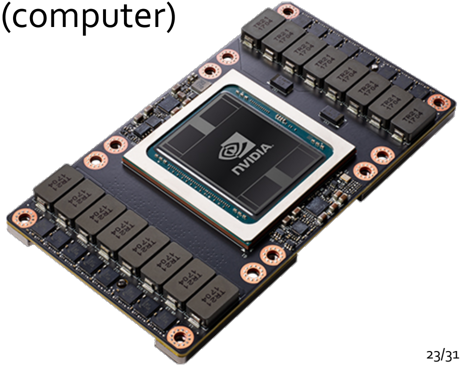
GPU utilization

GPU utilization

GPUs are an expensive resource compared to CPUs (× 60 BUs!)
→ GPU should be maximally utilized!

For a running job:

- use `squeue` to find out on what node (computer) it is running
- ssh into that node, e.g., `ssh r01g01`
- find the process id of your job with `ps -u $USER`
- run `nvidia-smi`



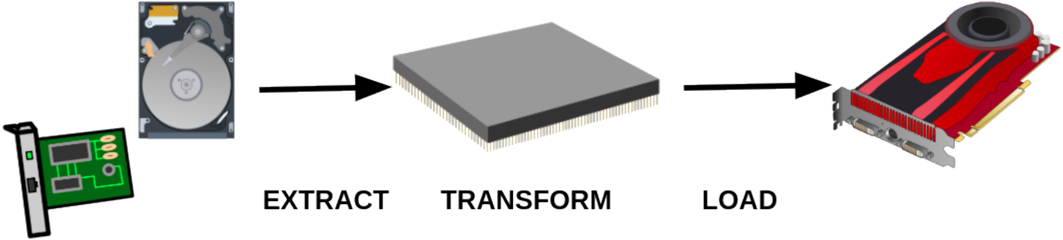
GPU utilization

For a finished job:

- run `gpuseff <jobid>`
- shows GPU utilisation statistics for the whole running time
- note: gpuseff is currently in testing usage, and still under development

You can always contact our service desk if you need advice on how to improve your GPU utilization!

Using multiple CPUs for ETL



- Common bottle-neck: CPU cannot keep up with GPU
- GPU has to wait for more data ...
- Solution: use more CPUs (they are “cheaper” than GPUs!)

A good rule of thumb in Puhti is to reserve 10 CPUs per GPU (as there are 4 GPUs and 40 CPUs per node).

Using multiple CPUs for ETL

In Slurm scripts:

```
#SBATCH --cpus-per-task=10
```

Note: using multiple CPUs *not* automatic, code needs to support it!

For example in TensorFlow:

```
dataset = dataset.map(..., num_parallel_calls=10)
dataset = dataset.prefetch(buffer_size)
```

PyTorch:

```
train_loader = torch.utils.data.DataLoader(..., num_workers=10)
```

Multi-GPU and multi-node jobs

Multi-GPU

Many frameworks support multi-GPU within a single node.

Slurm script:

```
#SBATCH --gres=gpu:v100:4
```

TensorFlow:

```
mirrored_strategy = \
  tf.distribute.MirroredStrategy()
with mirrored_strategy.scope():
    model = Sequential(...)
    model.add(...)
    model.add(...)
    model.compile(...)
```

PyTorch:

```
model = MyModel(...)
if torch.cuda.device_count() > 1:
    model = nn.DataParallel(model)
model.to(device)
```

Multi-GPU and multi-node

- A single node has 4 GPUs
- If you need more than 4 GPUs, we recommend Horovod
- Supported for TensorFlow and PyTorch on Puhti
- Uses MPI and NCCL for interprocess communication
- Modules with `-hvd suffix`

Try:

```
module avail hvd
module load tensorflow/2.0.0-hvd
```

Slurm example for Horovod

Example slurm script that uses 8 GPUs across two computers

- MPI terminology: 8 tasks, 2 nodes
- Each task is 1 GPU and 10 CPUs

```
#!/bin/bash
#SBATCH --account=<project>
#SBATCH --partition=gpu
#SBATCH --ntasks=8
#SBATCH --nodes=2
#SBATCH --cpus-per-task=10
#SBATCH --mem=32G
#SBATCH --time=1:00:00
#SBATCH --gres=gpu:v100:4

srun python3 myprog.py <options>
```

Singularity containers