THE UNIVERSITY *of* EDINBURGH
informatics

Using GPUs for NLP in Informatics

Doing Research in Natural Language Processing
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11/13 October 2023

Overview

- GPUs in Machine Learning
- Working with GPUs
- What is a cluster and slurm
- When to use a cluster
- How to access and use it
- Walkthrough running experiments
- Resources for workflow
- Getting help
- Demo + Tutorial on the ILCC cluster (Friday!)

Reading the room

- ✅ I’m comfortable with shells/bash, SSH and remote access
- ✅ I am comfortable writing my own experimental code
- ✅ I know how to use CUDA and run GPU experiments
- ✅ I have used a cluster (any cluster) before
- ✅ I have used a Slurm managed cluster before

GPUs in Machine Learning

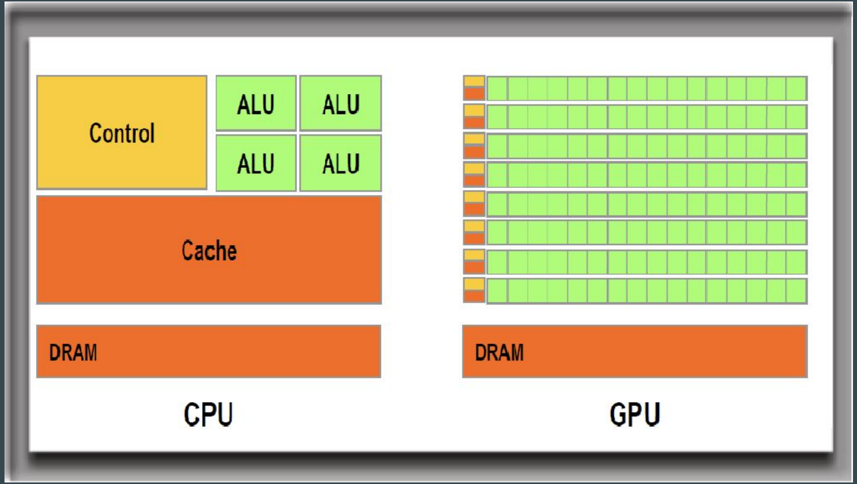
Machine Learning demands many calculations

```
>>> import torch

>>> a = torch.randn((1024,512))

>>> b = torch.randn((2048,1024))

>>> torch.matmul(b,a)

# Approximately 1B operations!
```

- CPUs have few, high power processing cores
- On a CPU, each product must be calculated sequentially leading to slow processing.
- But each operation is a simple instruction so can this be sped up?
- Can we delegate processing to many smaller processing cores?

What is a GPU?

- GPUs enable rapid parallel processing of operations.
- Many small cores working in parallel rather than a few large CPU cores.
- ~4300 cores means less concurrency constraints!
- Useful for graphical tasks and gaming but now a must-have tool for Machine Learning and Scientific Computing.

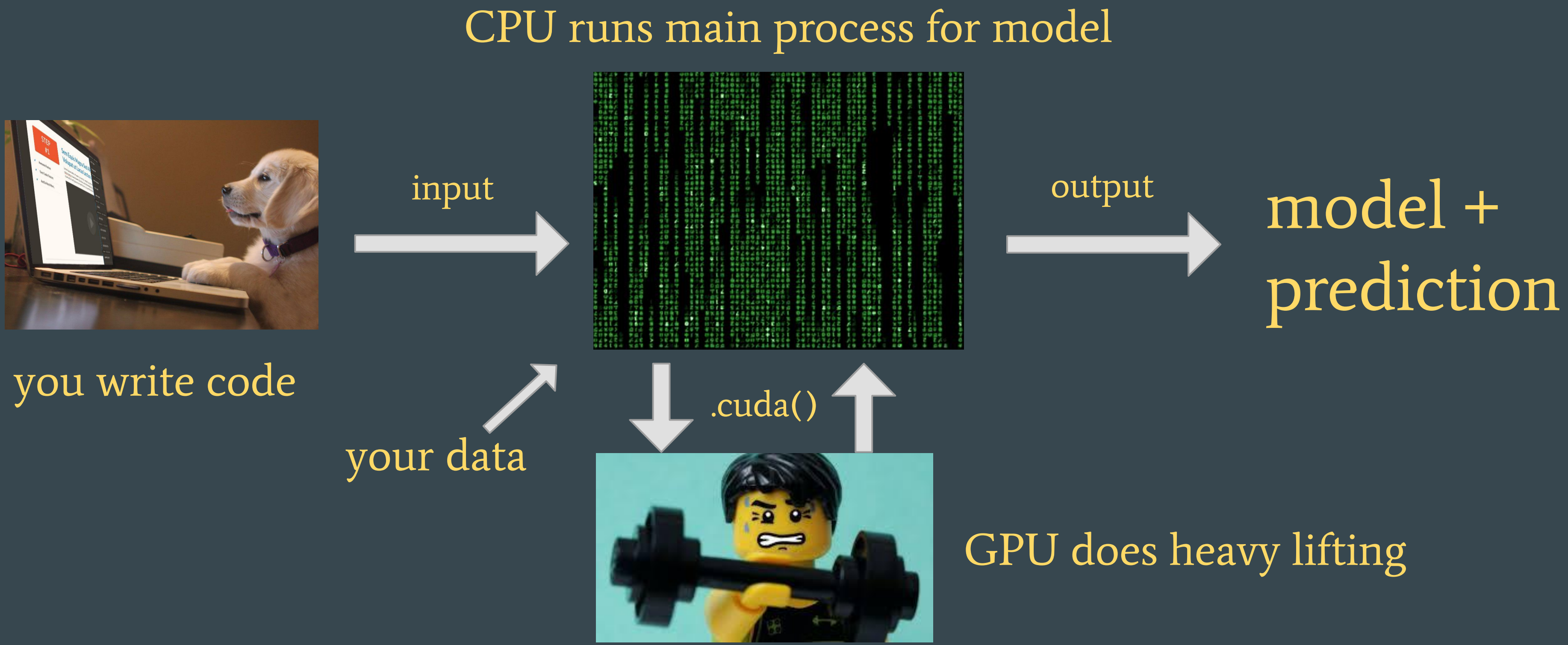


Working with GPUs

```
>>> import torch
>>> a = torch.randn((1024,512))
>>> b = torch.randn((2048,1024))
>>> torch.matmul(b,a)
7.39s to compute 1000x
>>> a = a.cuda()
>>> b = b.cuda()
>>> torch.matmul(b,a)
2.36s to compute 1000x
```

- We use the NVIDIA CUDA interface to integrate GPUs into our code.
- All our code today is in PyTorch which plugs into CUDA without us writing GPU instructions. Other options exist if desired.
- Write code as normal then move matrices to the GPU for speed up.
- GPUs have their own memory.
    - Small models fit entirely on a GPU (not ~~BERT~~Llama!)
    - Or process data through a GPU model in batches.
    - Need multiple GPUs? We will look at this later...

Workflow of using a GPU in NLP



A typical experiment outline

```
#!/bin/bash
1.   Create folders, check data
     and environment

2.   Train model using GPU

3.   Generate predictions and
     scores from test set

4.   Cleanup from experiment

5.   Done!
```

- A model training experiment can be automated into a shell-script to complete setup, training, inference and cleanup.
- This is for after model development, when you are confident that your model operates as intended.
- Formatting your experiments as a script makes migrating to clusters easy!

What is a cluster?

What is a cluster?

- An arrangement of servers to execute computationally intensive work on dedicated high-performance machines in the background.
- You log into the head node, format your experiments and then submit scripts as “jobs”.
- Your jobs are assigned a compute node (with a GPU) which runs your script and accesses a shared or local file system for data.
- Jobs are assigned, managed and controlled using a scheduler program.
  Informatics uses the Slurm scheduler.

Why use a cluster?

Single GPU experiments

- ✅ Debug models during development with direct shell access to model e.g. using PDB
- ❌ GPU also required to run monitor and other processes.
- ❌ One experiment at a time.
- ❌ Computer possibly not usable during experiments.

Cluster experiments

- ❌ No direct access to shell. Hard to debug errors .
- ✅ GPU dedicated to your experiment.
- ✅ Run many parallel experiments.
- ✅ Sharing GPUs maximises usage without grinding your own PC to a halt.

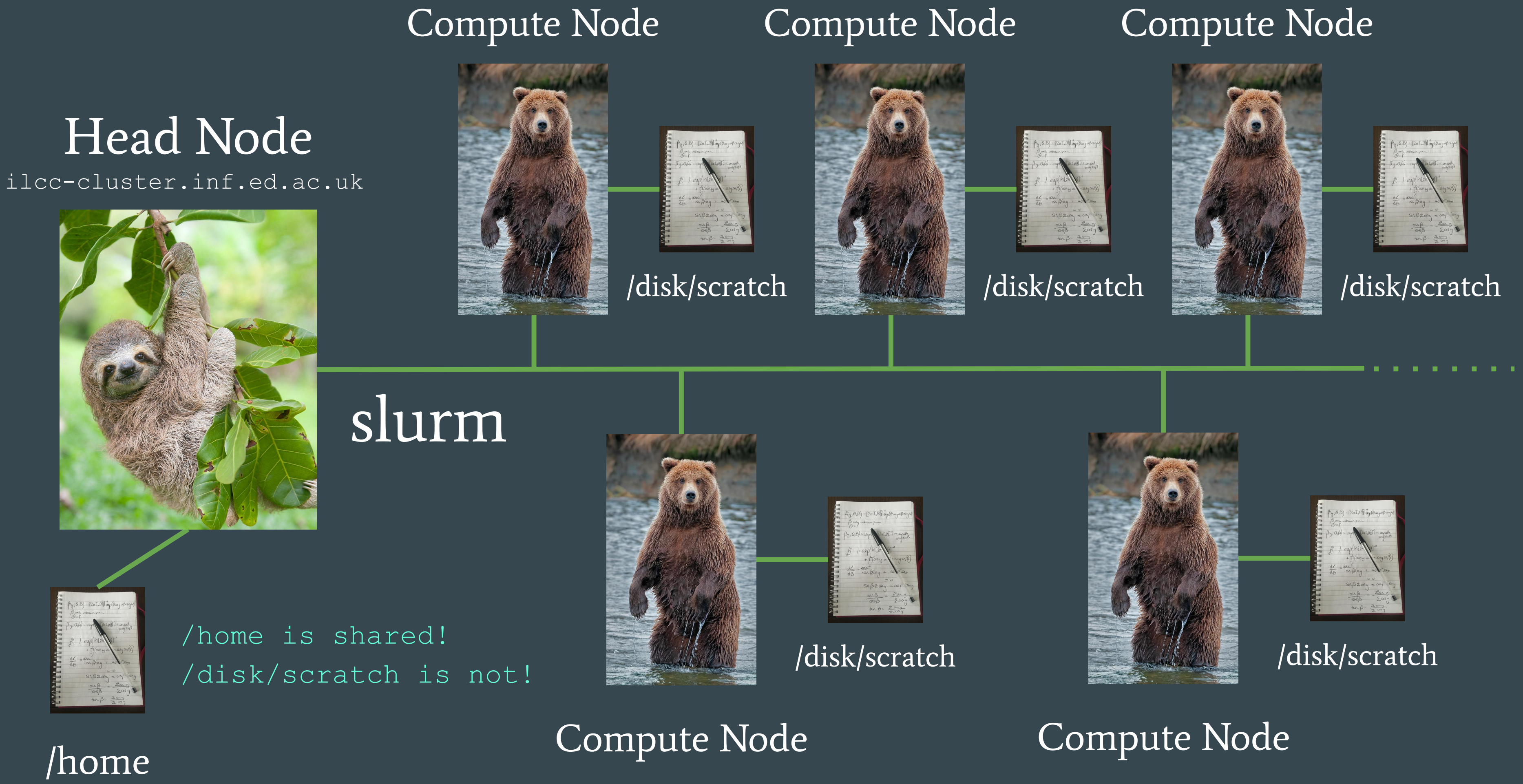
What do we have in Informatics?

- ILCC cluster: `ilcc-cluster.inf.ed.ac.uk / escience6`
  - ~80 GPUs for your work across various machines. CDT students have their own partition.
  - A combination of NVIDIA RTX2080 Ti / NVIDIA RTX1080 Ti cards with 11GB memory.
  - One very large storage disk (`ostrom`) connected by NFS.

- PGR Cluster: `mlp.inf.ed.ac.uk / uhtred`
  - `Crannog[01-07]` each has 4xA40s (48GB memory) + 510 GB RAM
  - `Damnii[1-12]` each has 7/8 RTX 2080s (11 GB memory) + 190GB RAM
  - 123 GPUs for use between all PGR students.
  - Other partitions (e.g., `Teach-Standard`) are used by others and sometimes shared.
    e.g., `landonia` machines have some A6000s.

- EIDF is a new resource to be demo'd in Second Semester (uses a Docker/Kubernetes system)

- Some CDT-NLP students will refer to CSD3. This is no longer available through the CDT



```
/home is shared!
/disk/scratch is not!
```

Disk spaces on the cluster

- Like DICE, you will have a home folder as `/home/${USER}/`
- Move data between machines using `rsync` or `scp`.
- Your user space is on a network disk that all nodes can access.
  - `/home/` is actually `/disk/nfs/ostrom`
  - 168TB disk shared between all users. Keep results and environments here.
  - This disk is large but also slow.
  - There are no backups! Got important work? Copy it out of the cluster.

- Each compute node has a local disk drive at `/disk/scratch/`
  - This is fast to read and write to during an experiment.
  - Save weights and large file here during training.
    - Copy what you need back to your user space at the end.
    - Delete everything else you haven't stored from here at the end.

What is Slurm?

- Slurm is an open source scheduler that controls the allocation and execution of jobs on our cluster.

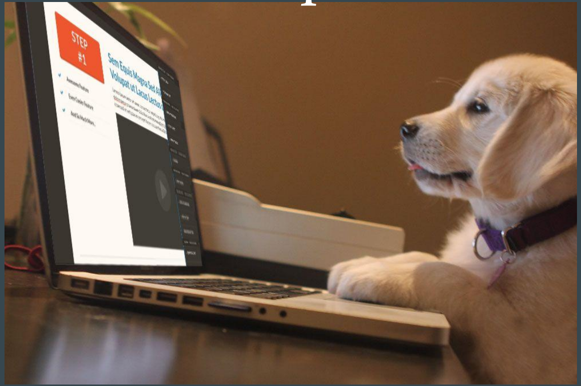
- You write your experiment script then...
  - You submit your script to the Slurm controller while logged into the head node.
  - Slurm finds an available compute node and assigns resources to execute your script.
  - You can monitor your job output and status using Slurm monitoring commands.
  - No free compute node? Slurm places your jobs in a queue to execute when a GPU is free.

Slurm commands

- `sbatch` - submit a job for hands-off execution on the cluster.
- `srun` - request an interactive shell session on a compute node (for debugging)
- `squeue` - check the execution of your jobs and the queue of waiting jobs
- `sinfo` - check cluster information
- `scontrol` - update job configuration (won’t be covering today)

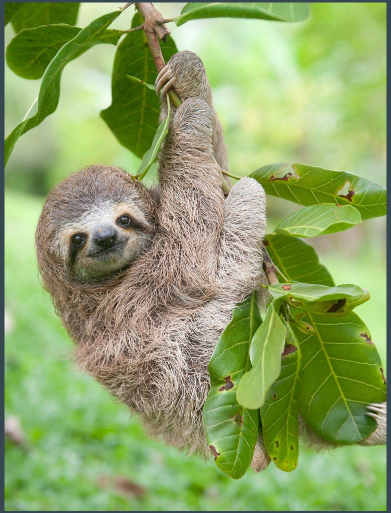
Use ssh to access the head node

Local computer



ssh →

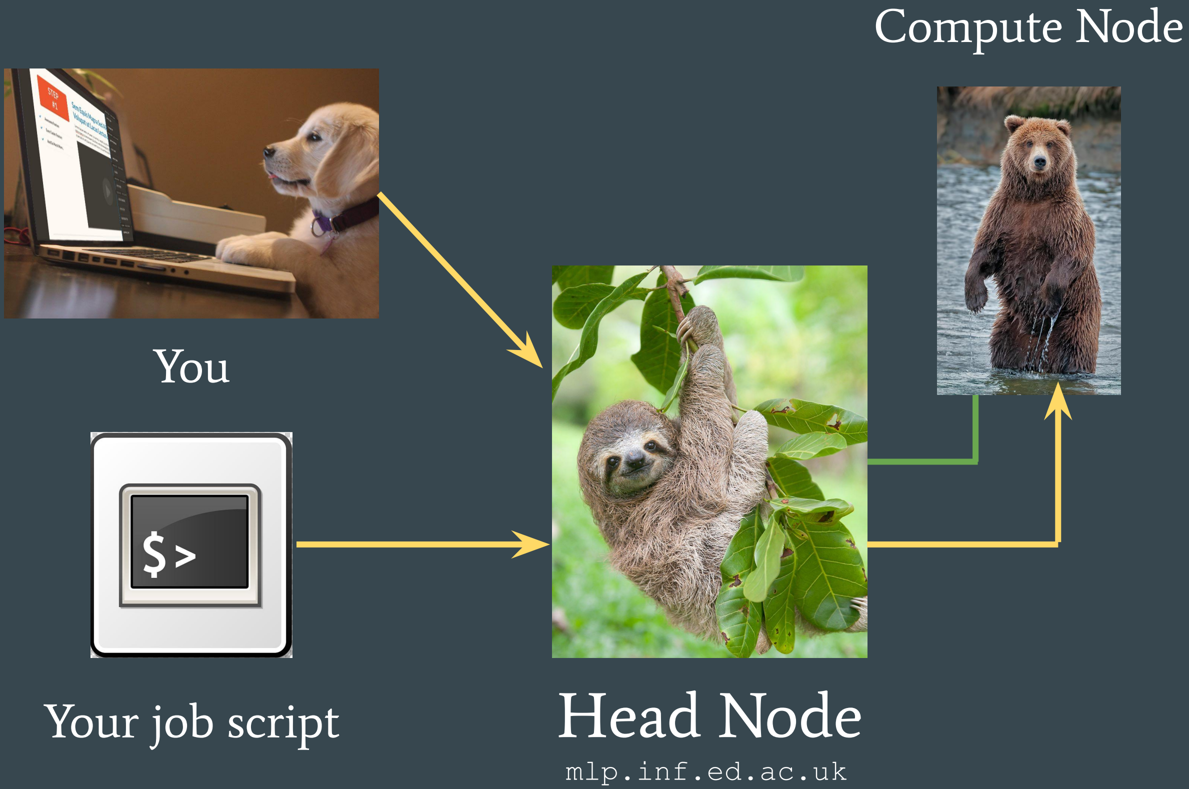
Head Node



For example:

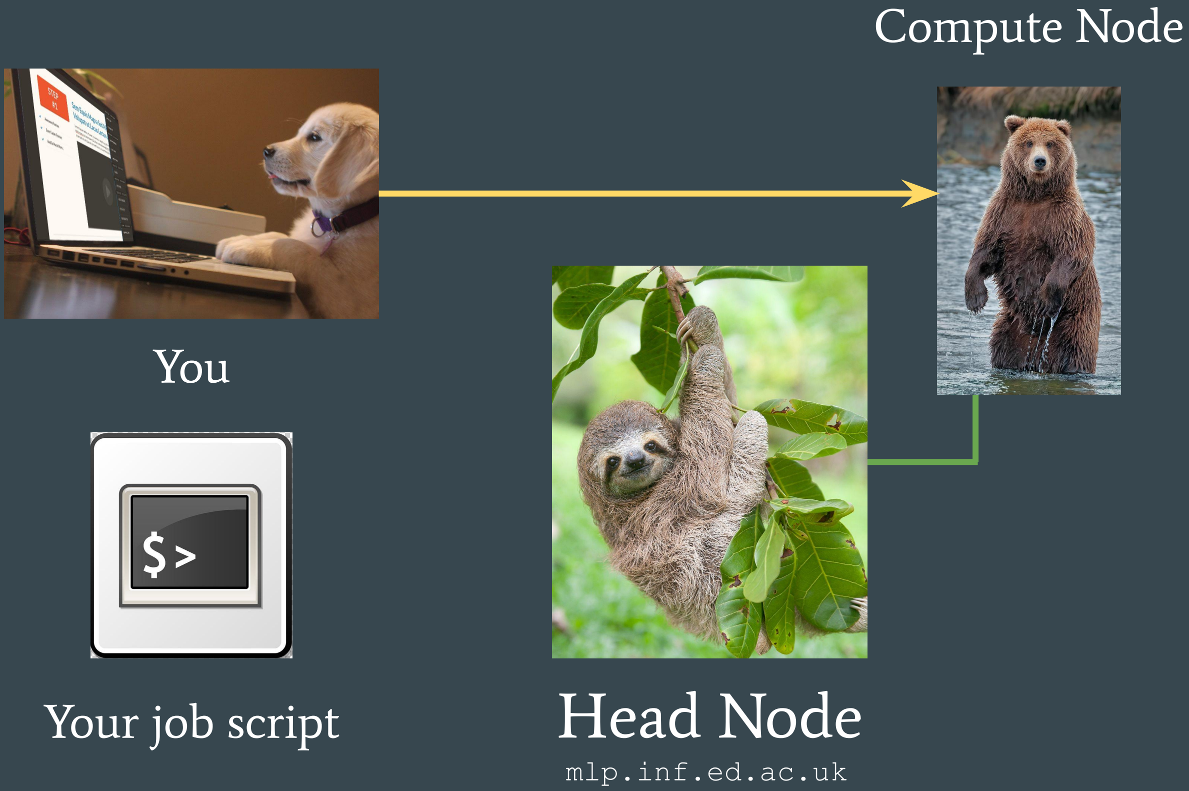
```
    ssh ${USER}@ilcc-cluster.inf.ed.ac.uk
    ssh ${USER}@mlp.inf.ed.ac.uk
    ssh ${USER}@${cluster_name}.inf.ed.ac.uk
```

`sbatch`



- You SSH onto the head node.
- Submit your job using `sbatch`.
- Slurm assigns the job to a compute node and then executes the job in the background.

`srun`



- Slurm assigns you an interactive session on the compute node (like SSH)
- Useful if your job is going wrong somewhere/debugging.
- No automatic processing and job is not a background process.

Comparing sbatch and srun

`sbatch`

- ✅ Your experiment runs as a background process without direct supervision.
- ✅ Run all your experiments in parallel on compute nodes.
- ✅ The intended use case for cluster computing.
- ✅ Go home and rest. Your work is happening while you sleep!

`srun`

- ✅ Gives you an SSH-like session on a compute node. Useful if something has gone wrong and you need to check your model on the cluster.
- ❌ Hoards GPU resources if used excessively.
- ❌ The cluster becomes less useful and effective.
- ❌ Encourages poor experiment design and babysitting your jobs.

Everything all together...

- Assume that experiments are bash scripts that specify all steps of computation.
- We access a cluster by SSHing on to the head node.
- Submit an experiment job using `sbatch` to request a compute node to run the job.
- Slurm manages the allocation, execution and running of jobs.

Cluster Workflow

Anatomy of an `sbatch` script

```
#SBATCH Args here....
```

```
conda activate pt
```

```
rsync data /home/ to /disk/scratch/
```

```
python train.py
```

```
python predict.py
```

```
rsync results /disk/scratch/ to /home/
```

```
rm -rf /disk/scratch/${USER}/exp
```

You will need...

- Slurm configuration
- A Python environment
- Training and test data
- The model to train (`model.py`)
- Training command (`train.py`)
- Prediction command (`predict.py`)

Conda Environments

- Miniconda provides isolated runtime environments for your Python code. This manages your packages so you can be sure what dependencies you are using in your programme.

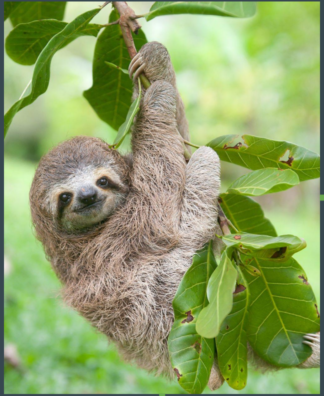
- Install a specification of packages to an environment and use it for all your experiments!

- Different experiments have different specifications? Use a new environment!

- We will install tools such as PyTorch in an environment.

Data transfer

Head Node



1

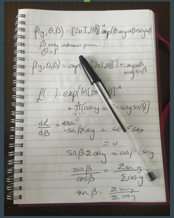
input data -> compute node scratch

Compute Node processing

2

DFS <- results from compute node scratch

3

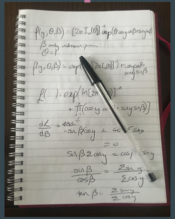


git + results

miniconda

input data

/home/ logs



results

input data

scratch

Software to use

>scp

rsync

Git Large File Storage

```
$ wget
```

Moving data

ANACONDA®

Package management
& virtual environments

Version control

git

&

GitHub

Writing code

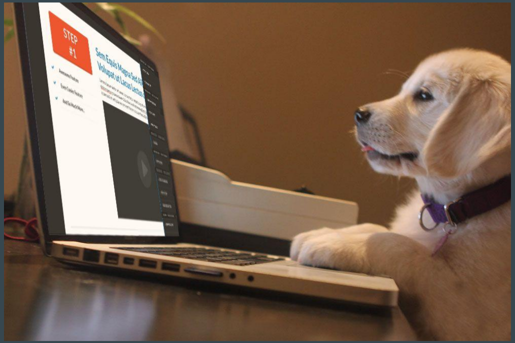
jupyterlab TNG

Vim

Experiment checklist

- ✅ A working model pushed to GitHub (or other VCS) to clone from
- ✅ Code and data in my `/home/$USER/` folder on the shared file system
- ✅ A `conda` environment to run my Python code within
- ✅ I know how much RAM and GPUs I need
- ✅ Bash script defining the stages of the experiment, config and data transfer.

Local Computer

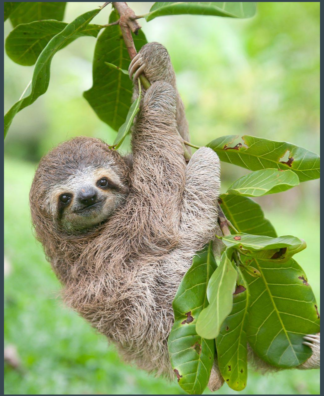


ssh

1. Write your code and get it working with a conda virtual environment

2. Version control your code with git and put it in a repository online with GitHub

Head Node



slurm

3. Download your code by cloning repo from GitHub

4. Create/activate conda environment.

5. Get your input data onto the DFS e.g. scp / rsync

8. Run <u>YOUR JOBS</u> with sbatch

Compute node

6. Test your code on an srun interactive session

7. Last minute code edits on command line editors like vim or emacs

Now what?

Getting help

- `#computing` channel in the CDT in NLP slack
  - Peer support from other cluster users
  - Also useful if you want to help other people out!
  - (Note: I am not in this slack.)
- Ask your research group
  - Most senior-ish PhD students have got the hang of the cluster.
  - Most of us are happy to help share our knowledge.
- Submit Tickets to Computing Support 🎫
  - Try and be as specific as possible.
    What do you think is the error?
    Is it reproducible?
    What Slurm job # caused this?

Cluster etiquette

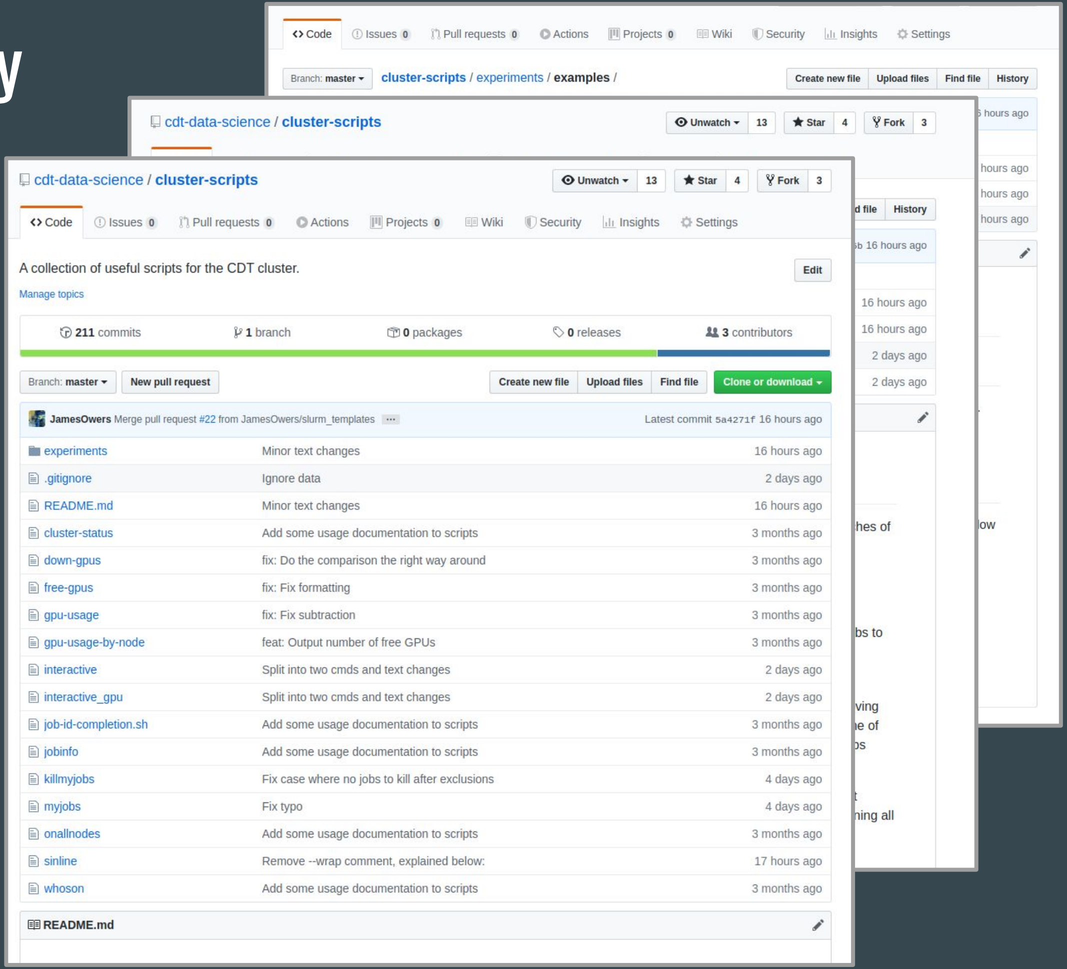
- Be nice!
- Running a lot of jobs? Consider staggering so many users can use the queue
- Or use Array jobs (not covered today but included in the demo)
- If you see someone misbehaving then consider emailing them (they may be unaware)
- Similarly, another user may notify you if they see a process of yours acting improperly (e.g. running Python on the head node)

The cluster-scripts repository

Repo here:
https://github.com/cdt-data-science/cluster-scripts

1. scripts to make your life easier
2. examples for quick learns
3. templates for running experiments fast

We will use this in today's demonstration!



Code · Issues 0 · Pull requests 0 · Actions · Projects 0 · Wiki · Security · Insights · Settings

Branch: master · cluster-scripts / experiments / examples /

cdt-data-science / cluster-scripts

cdt-data-science / cluster-scripts

Unwatch 13 · Star 4 · Fork 3

A collection of useful scripts for the CDT cluster.

Manage topics

211 commits · 1 branch · 0 packages · 0 releases · 3 contributors

Branch: master · New pull request · Create new file · Upload files · Find file · Clone or download

JamesOwers Merge pull request #22 from JamesOwers/slurm_templates · Latest commit 5a4271f 16 hours ago

experiments	Minor text changes	16 hours ago
.gitignore	Ignore data	2 days ago
README.md	Minor text changes	16 hours ago
cluster-status	Add some usage documentation to scripts	3 months ago
down-gpus	fix: Do the comparison the right way around	3 months ago
free-gpus	fix: Fix formatting	3 months ago
gpu-usage	fix: Fix subtraction	3 months ago
gpu-usage-by-node	feat: Output number of free GPUs	3 months ago
interactive	Split into two cmds and text changes	2 days ago
interactive_gpu	Split into two cmds and text changes	2 days ago
job-id-completion.sh	Add some usage documentation to scripts	3 months ago
jobinfo	Add some usage documentation to scripts	3 months ago
killmyjobs	Fix case where no jobs to kill after exclusions	4 days ago
myjobs	Fix typo	4 days ago
onallnodes	Add some usage documentation to scripts	3 months ago
sinline	Remove --wrap comment, explained below:	17 hours ago
whoson	Add some usage documentation to scripts	3 months ago

README.md

Common mistakes

- Conda environment not set up properly to use a GPU.
  - Check `torch.cuda.is_available()==True` in an interactive session.
- Training fails due to Out Of Memory errors.
  - Consider adjusting batch sizes to reduce peak GPU memory.
  - Or reformat your model to use multiple GPUs.
- Nothing happens when I submit using `sbatch`?
  - Check your `sbatch` arguments. `sbatch` will fail **silently** if the arguments contain an error
    - e.g., `--parition=illc-cluster`
- My job stops after a few seconds
  - The `/disk/scratch` of a compute node might be full. Identify the node and submit a ticket!

Not covered today

- Using EIDF cluster:
  - Many GPUs and resources but an entirely different experiment paradigm.
  - To be explained in Semester 2
- CSD3 Cluster:
  - No longer supported by CDT. You may get access through your supervisor.
- Multi GPU jobs:
  - Used to be much more complex but now tools like HuggingFace Trainer / Mosaic Composer can seamlessly use all available GPUs.
- Using singularity in a Slurm job:
  - Computing Support have a help page for this: https://computing.help.inf.ed.ac.uk/singularity
- Using Array jobs
  - An example of this is in the Demo on Friday

Demonstration

- Cluster Scripts
- Setting up a workspace
- Experiment walkthrough