Python on Trillium and Open OnDemand

Ramses van Zon

October 27, 2025

In this workshop...

- Why Python?
- Why Supercomputers?
- Access
- Using Trillium
- Installing packages
- More about OnDemand

Why Python?

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- But the interpreted and dynamic nature of Python is often at odds with "high performance". **Yes, Python itself is slow!**
- This matters a lot less when Python is the 'driver' or 'glue language' for optimized packages or programs, such as for AI and ML.

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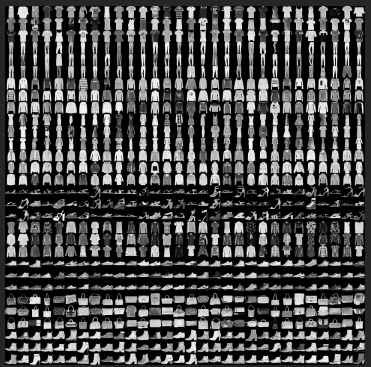

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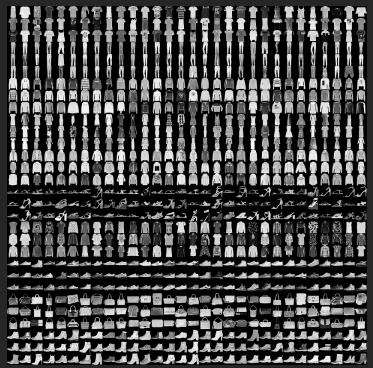

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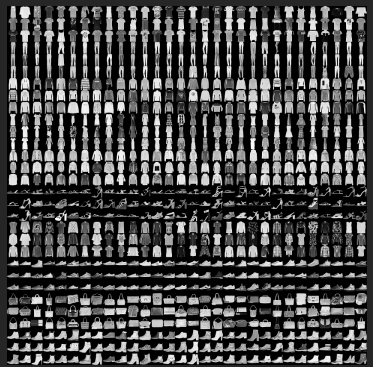

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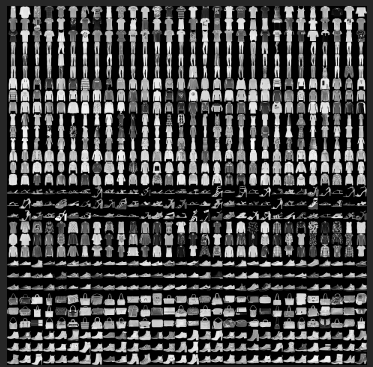

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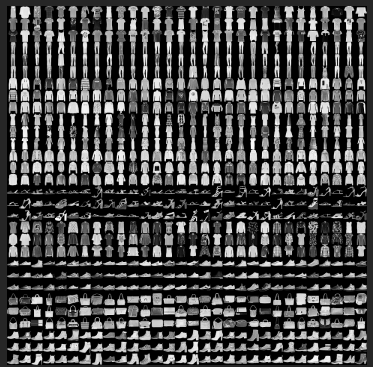

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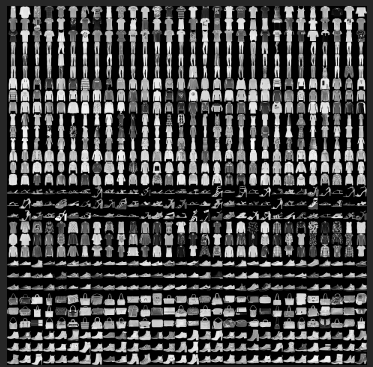

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Although this example would be too small to warrant running on the Trillium supercomputer, it will demonstrate many aspects of running Python applications on such a system.

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Congratulations, you are now doing Advanced Research Computing!

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Getting started

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You can learn a lot more about using Trillium than we will cover today, in the self-guided course "Intro to Trillium", see https://scinet.courses/1389.

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- You can now go to "Clusters; Trillium Shell Access" to get a command line on one of the Trillium login nodes.

Hands-on 1

Hands-on 1 (5 min)

Get logged into Trillium by one of these two methods.

Then, type the command

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(and press Enter).

It should say:

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Note: The dollar sign ("$") in the slides will be an abbreviation of the full prompt, which will look more like `[rzon@tri-login01 ~]$`.

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Need to brush up on the Linux command line? SHARCNET has a self-guided course for that: https://training.sharcnet.ca/courses/enrol/index.php?id=182.

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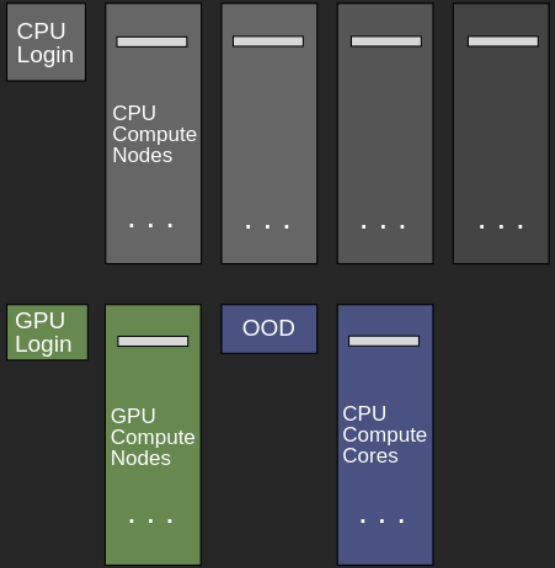

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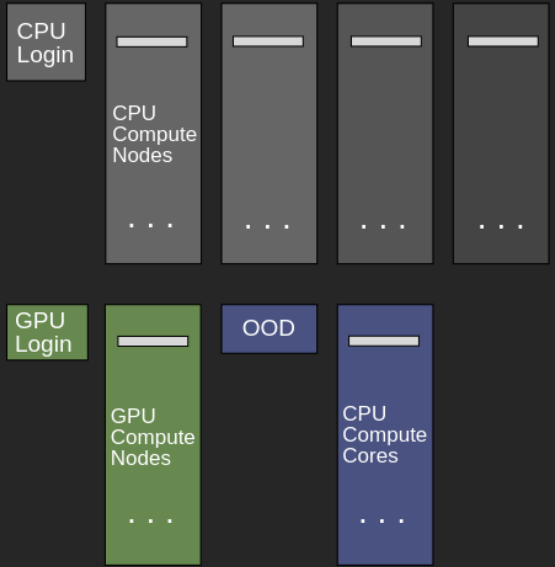

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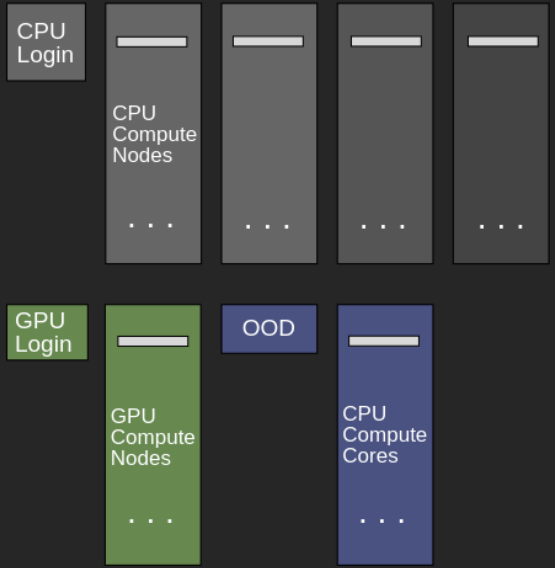

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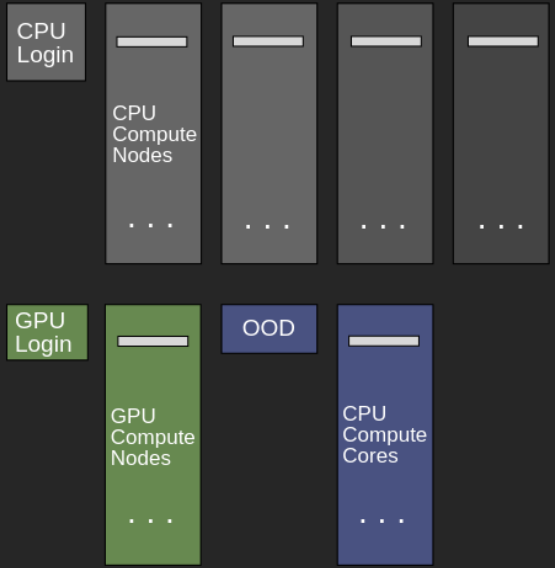

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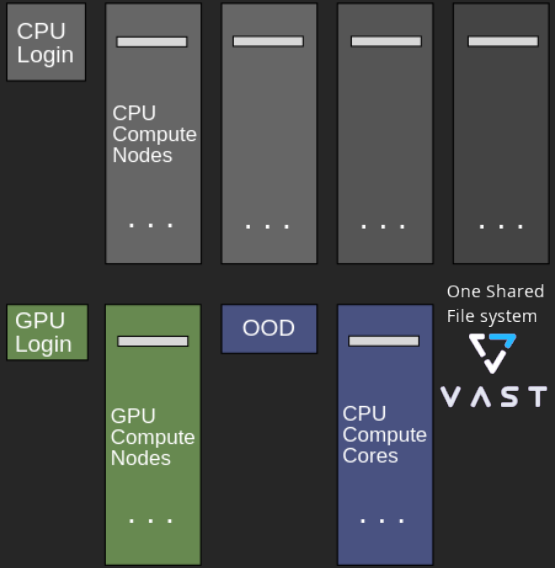

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Hands-on 2

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- From a CPU login node, copy the python code in /home/rzon/fashion.py to your own directory.
- Try to run it with `python fashion.py`; it should fail.
- Try `pip install torch`. What does it do? Does it work after that?

Why not?

Software packages

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- A little utility called `mii` would have found a number of versions of `pip`.
- If you selected one, pip would install it for that version.was tied to a specific python module.
- Pip installed the package in `$HOME/.local/lib/pythonVERSION/site-packages`.

But since we did not load that python module, so `python fashion.py` failed.

Bad solution: only load a module

If you do `module load python/VERSION`, it would work now.

But what if you yourself need to use different sets of packages?

Good solution: Use a virtual environment

```
$ module load python/3.13
$ virtualenv --no-download ~/.virtualenvs/myenv
$ source $HOME/.virtualenvs/myenv/bin/activate
(myenv) $ pip install --no-index torch
```

Hands-on 3

Hands-on 3 (10 minutes)

- Create the virtual environment. You will also need the package `torchvision`, so:

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(myenv) $ pip install --no-index torch torchvision
```

- By the way, the options `--no-downloads` and `--noindex` cause this procedure to only use optimized packages from the wheelhouse.*
- What pip installed in the default directory, would override the ones in the virtual environment, so remove that:

```
$ rm -rf $HOME/.local/lib/python*/site-packages
```

- Make sure `python fashion.py` now starts properly.

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- Make sure `python fashion.py` now starts properly.
- And see what fails next.(really? sorry yeah, really.)

To the compute nodes!

```
(myenv) $ python fashion.py
CPU time limit exceeded
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- We ran this on a CPU login node, a **shared resource**.
- For fairness, each user can only run a limit amount of time.

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Caveat (again)! This task here is not really heavy enough to warrant using a full 192-core Trillium node!

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So:

1. Bundle up short and small jobs (beyond today's workshop).
2. Write a job script to be submitted to the scheduler.
3. Fine, but we can get emails when the job starts and ends.
4. Copy everything for a job to $SCRATCH
5. Write a separate python script to download the data (or run once from the login node).

Hands-on 4

Hands-on 4 (20 min)

- Setup a directory in scratch:

```
(myenv) $ mkdir $SCRATCH/myrun
(myenv) $ cp fashion.py $SCRATCH/myrun
(myenv) $ cd $SCRATCH/myrun
```

Hands-on 4 (20 min)

- Setup a directory in scratch:

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(myenv) $ mkdir $SCRATCH/myrun
(myenv) $ cp fashion.py $SCRATCH/myrun
(myenv) $ cd $SCRATCH/myrun
```

- Download the data from the login node:

```
(myenv) $ python
>>> from torchvision import datasets
>>> training_data = datasets.FashionMNIST(root="data",download=True)
>>> exit()
```

Hands-on 4 (20 min)

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```
(myenv) $ python
>>> from torchvision import datasets
>>> training_data = datasets.FashionMNIST(root="data",download=True)
>>> exit()
```

- Create a jobscript and submit it:

```
(myenv) sbatch -pdebug jobscript
```

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=192
#SBATCH --time=0:16:00
#SBATCH --mail-type=ALL
#SBATCH --mail-user=rzon@...
#SBATCH --output=jobscript_%j.out
module load python/3.13
source $HOME/.virtualenvs/myenv/bin/activate
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
python -u fashion.py
```

GPUs, you ask?

Yes, of course, AI workload such as this should run on GPUs.

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- log into the gpu login node

```
(myenv) $ ssh trig-login01
$ module load python/3.13
$ source $HOME/.virtualenvs/myenv/bin/activate
(myenv) $ cd $SCRATCH/myrun
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- and adapt the jobscript to ask for a GPU

```
$ cp jobscript jobscriptgpu
$ nano jobscriptgpu
```

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(myenv) $ cd $SCRATCH/myrun
```

- and adapt the jobscript to ask for a GPU

```
$ cp jobscript jobscriptgpu
$ nano jobscriptgpu
```

```
#SBATCH --gpus-per-node=1
#SBATCH --cpus-per-task=24
```

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```
$ cp jobscript jobscriptgpu
$ nano jobscriptgpu
```

```
#SBATCH --gpus-per-node=1
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```

Note that in jobscript, and when we ssh into another login node, the virtual environment is no longer active and modules are not loaded; you must reload and reactivate.

Hands-on 5

Hands-on 5 (5 min)

Let's run it on the GPU subcluster of Trillium!

Okay, but what about interactive notebooks?

SciNet's Open OnDemand

Not everything needs 192 cores, or a GPU

What if you have that one postprocessing step that you need less than 192 cores for? What if you need to do some visualization?

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SciNet installed the OnDemand to provide Jupyter Lab and other features in the browser.

Logging into the Open OnDemand portal

To access the Open OnDemand portal, open a web browser and navigate to the following page:
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From here you can access the various tools and applications available on the platform.

File management

The Open OnDemand platform provides a file browser.

Click on the **Files** tab and select which directory you want to manage from the drop-down (`HOME`, `SCRATCH` or `PROJECT`).

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Note: there is a Globus button in the file browser at the top right as well, which will take you to the Globus web interface.

Interactive applications

Perhaps the most convenient part of Open OnDemand are its interactive applications that can be run directly from your web browser. To access the applications, navigate to the ***Interactive Apps*** tab and select the application you want to run from the drop-down.

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The application will open in a new tab in your browser.

Available applications in OnDemand

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- Trillium Desktop - a graphics desktop in your browser
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- ARM Forge - to use the parallel debugger DDT
- and last but not least: **Jupyter Lab**.

Jupyter Lab

We have two flavours of this:

- The default ‘native’ Jupyter Lab
- JupyterLab with Alliance software extensions. These can give you similar applications to the OOD interactive applications, but started from Jupyter.

We’ll use the first here.

Hands-on 6

Hands-on 6 (5 minutes)

Part 1: * Access OpenOnDemand * Start a Jupyter Lab session with 4 cores, 8 GB, for 1 hour. * Go to the Launcher tab.

But you won't see your 'myenv' environment?

VENV2JUP

This is an essential utility to make your virtual environments visible in the JupterHub.

In a terminal (possibly the one on OpenOnDemand):

- Load all needed modules

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In a terminal (possibly the one on OpenOnDemand):

- Load all needed modules
- Activate your environment
- And run

```
(myenv) $ venv2jup
```

This installs some packages and puts a file in `$HOME/.local/share/jupyter/kernels`, which is how the JupyterLab knows it exists.

Hands-on 7

Hands-on 7 (5 minutes)

- Perform the venv2jup step.
- Refresh the jupyter lab interface.
- Start a 'myenv' notebook.
- Check that it works with "`import torch`'

Thank you for your attention!