Python on Trillium and Open OnDemand

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October 27, 2025

In this workshop. . .

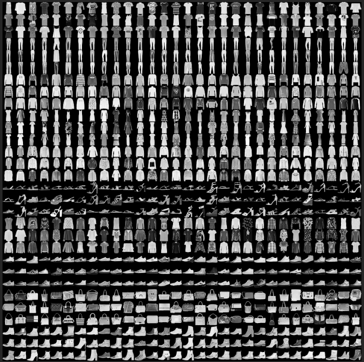
- Why Python?
- Why Supercomputers?
- Access
- Using Trillium
- Installing packages
- More about OnDemand

Why Python?

Python is great

- Python is a high-level, interpreted language.
- Python is fairly easy to learn, very expressive, and, not surprisingly, very popular.
- Its greatness is in large part due to the available packages.
- And in its interactive computing paradigm (=> Jupyter Lab)
- Development in Python can be substantially easier (and thus faster) than when using compiled languages.
- 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.

Running example



- We have a data set of images of fashion items, (“T-shirt/top”, “Trouser”, “Pullover”, “Dress”, “Coat”, “Sandal”,“Shirt”, “Sneaker”, “Bag”, “Ankle boot”):
  See: https://github.com/zalandoresearch/fashion-mnist
- We want to train an artificial neural work on this data set so we could recognize items in other images.
- We’ll use PyTorch for this task.

This use case was taken from a PyTorch tutorial:
https://docs.pytorch.org/tutorials/beginner/basics/quickstart_tutorial.html

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.

Why use a supercomputer?

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Your research project may need more resources than your laptop can provide.

This may be for several reasons:

1. Your research computations are too large to fit on your laptop.
2. The computations are too slow.
3. The computations are too plentiful.

So you go to one of the Alliance's 'advanced research computing' clusters: like Nibi, Fir, Narval, Rorqual and Trillium.

Congratulations, you are now doing Advanced Research Computing!

Advanced Research Computing

A supercomputer is just like your laptop

Haha! You didn't really think so, right?

We are going to need to make some adjustments.

Using a supercomputer is different

1. It is remote.
2. It's usually command-line driven.
3. It is a shared resource.
4. It is not your own machine.

But it’s still got Python, right?

Well yes, but:

Many tutorials on Python, AI and ML assume that you are working on your own machine and have full privileges to reconfigure it (and mess it up).

We’ll show you how to operate in this shared space, focusing in particular on Trillium (but touching upon the other national systems as well).

When do we get to running Jupyter notebooks?

Patience, we’ll get there.

Getting started

Let's get onto Trillium!

What do you need to follow along this afternoon:

- An Alliance CCDB Account:
  https://ccdb.alliancecan.ca
- Setup MFA on CCDB
  https://ccdb.alliancecan.ca/multi_factor_authentications
- Access to Trillium (Resource -> Access Systems)
  https://ccdb.alliancecan.ca/me/access_systems
- Optional for today:
  - An ssh client;
  - Setup SSH keys. https://docs.alliancecan.ca/wiki/SSH_Keys

This will give you access to both Trillium terminal and SciNet's OnDemand service.

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.

Logging in

Option 1: Through an ssh client

Connects directly to the Trillium command line.

The supercomputer runs the remote **ssh server**. You local computer run the **ssh client**.

- Open a (local) terminal
- Type (uses SSH keys):

```
ssh USERNAME@trillium.alliancecan.ca
```

- Use your Yubikey or Duo app as 2nd factor.
- You now get a command line prompt on a Trillium login node.

Option 2: Through Open OnDemand

This is SciNet's **web interface** to Trillium meant for interactive applications.

OnDemand can also be used to get to the Trillium command line in your browser.

- Go to https://ondemand.scinet.utoronto.ca
- Log in with your CCDB USERNAME and password. (note: don't use your email).
- Use your Yubikey or Duo app as 2nd factor.
- 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

```
$ which python
```

(and press Enter).

It should say:

```
/cvmfs/soft.computecanada.ca/gentoo/2023/x86-64-v3/usr/bin/python
```

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

Command line

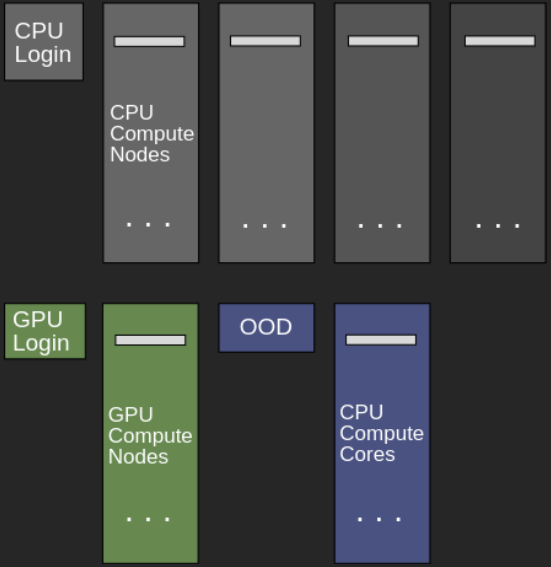
So we're always using this ~~~black screen of death~~~ command line?

Pretty much, yes, because

- In HPC and supercomputing, that's what people use.
- Any repetitive or large scale computational work requires working with the command line.
- Graphical User Interfaces (GUIs) would only offer existing functionality and GUI workflows are harder to automate or documents.
- Being familiar with the command line makes you more efficient, consistent, and productive in managing your data and your workflows.

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.

Understanding the Trillium system



Login nodes

- Ssh reaches the CPU or GPU login nodes.
- OnDemand reaches the OOD server.
- Shared among users
- Meant for preparing your work and software.

Compute nodes

- CPU: scheduled by 192-core node.
- GPU: scheduled by full NVIDIA H100 GPU.
- No internet access.
- Read-only home directory.

OOD compute cores

- Scheduled by core and memory
- Internet access.
- Writable home directory

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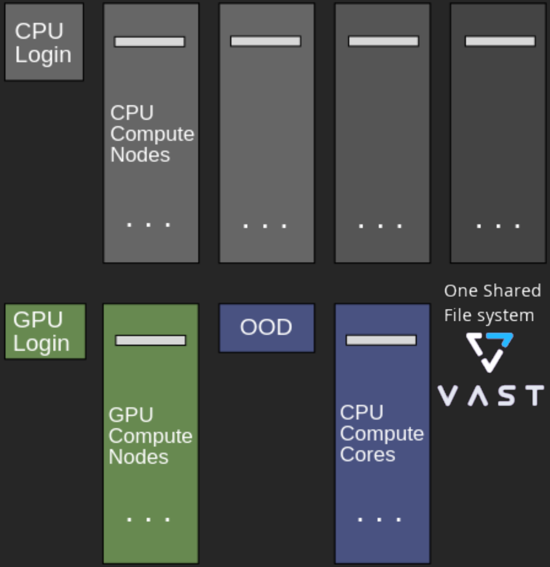

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Hands-on 2

Hands-on 2 (5 minutes)

- 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

It's a shared system

It is impossible to simultaneously install every user's required software and software version.

Almost all installed software is made available using modules

- These set environment variables (`PATH`, etc.)
- Allows multiple, conflicting versions of a given package to be available.
- `module overview [MODULE]` shows the available software.

Python wheels

- The module system does not work well for Python packages.
- One might try to just install these using `pip`, but you would get generic, non-optimized versions.
- To support optimized version of python packages, without requiring users to compile these themselves, we have a wheelhouse of packages that you can install into virtual environments.
- `avail_wheels [PACKAGE]` shows the available python packages.

Virtual environments

If you “pip installed”-ed `torch` in Hands-on 2, it did something:

- 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:

```
$ module load python/3.13
$ virtualenv --no-download ~/.virtualenvs/myenv
$ source $HOME/.virtualenvs/myenv/bin/activate
(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.
- And see what fails next.(really? sorry yeah, really.)

To the compute nodes!

```
(myenv) $ python fashion.py
CPU time limit exceeded
```

- We ran this on a CPU login node, a **shared resource**.
- For fairness, each user can only run a limit amount of time.
- For longer runs, you need to submit a job to run on the compute nodes.

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

Peculiarities of Trillium compute nodes

1. You always get a multiple of 192-core nodes (or a multiple of GPUs)
2. They run batch jobs through a scheduler
3. They run detached from a terminal
4. Cannot write to $HOME
5. No internet access

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
```

- Download the data from the login node:

```
(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.

Luckily, pytorch code can run on either a CPU or GPU dynamically.

We just have to:

- 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
```

- and adapt the jobscript to ask for a GPU

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

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

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?

For interactive work of that and other kinds in python, JupyterLab is typically used.

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

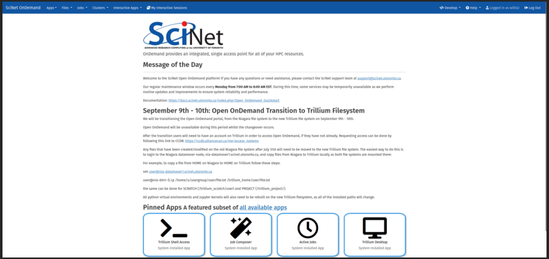
Logging into the Open OnDemand portal

To access the Open OnDemand portal, open a web browser and navigate to the following page: https://ondemand.scinet.utoronto.ca

You will be prompted to enter your Alliance username and password, followed by a second factor authentication via Duo or Yubikey.

Once you have logged in, you will be taken to the Open OnDemand dashboard.

From here you can access the various tools and applications available on the platform.



OnDemand provides an integrated, single access point for all of your HPC resources.

Message of the Day

Welcome to the SciNet Open OnDemand platform! If you have any questions or need assistance, please contact the SciNet support team at support@scinet.utoronto.ca.

Our regular maintenance window occurs every **Monday from 7:00 AM to 8:00 AM EST**. During this time, some services may be temporarily unavailable as we perform routine updates and improvements to ensure system reliability and performance.

Documentation: https://docs.scinet.utoronto.ca/index.php/Open_OnDemand_Quickstart

September 9th - 10th: Open OnDemand Transition to Trillium Filesystem

We will be transitioning the Open OnDemand portal, from the Niagara file system to the new Trillium file system on September 9th - 10th.

Open OnDemand will be unavailable during this period whilst the changeover occurs.

After the transition users will need to have an account on Trillium in order to access Open OnDemand, if they have not already. Requesting access can be done by following this link to CCDB: https://ccdb.alliancecan.ca/me/access_systems

Any files that have been created/modified on the old Niagara file system after July 31st will need to be moved to the new Trillium file system. The easiest way to do this is to login to the Niagara datamover node, nia-datamover1.scinet.utoronto.ca, and copy files from Niagara to Trillium locally as both file systems are mounted there:

For example, to copy a file from HOME on Niagara to HOME on Trillium follow these steps:

```
ssh user@nia-datamover1.scinet.utoronto.ca
```

```
user@nia-dm1:~$ cp /home/u/usergroup/user/file.txt /trillium_home/user/file.txt
```

the same can be done for SCRATCH (/trillium_scratch/user) and PROJECT (/trillium_project/).

All python virtual environments and Jupyter kernels will also need to be rebuilt on the new Trillium filesystem, as all of the installed paths will change.

Pinned Apps A featured subset of all available apps

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`).

You can:

- Navigate through your directories
- Upload/download files
- Create new files/directories
- Delete files/directories
- Edit existing files

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.

This will then bring you to the job submission page where you can choose job parameters such as:

- Length of job in hours
- Number of cores (there are no GPUs atm)
- Amount of memory to allocate (GB)
- Notify me by email when the job starts

When you have chosen your job parameters click on the ***Launch*** button to submit your job to the queue.

You will be taken to the ***My Interactive Sessions*** page where you can see the status of your job, i.e. queued, running or completed.

Once the job has been assigned a node and is running, you can click on the ***Connect to*** button to launch the application.

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

Available applications in OnDemand

- Trillium Desktop - a graphics desktop in your browser
- RStudio - an environment to run R
- VS Code - a code editor
- Paraview - a parallel visualization program
- 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
- 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!