A Technical Overview

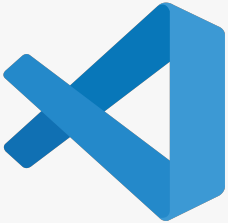
Romain Hermary

Friday 16th June, 2023

uni.lu
UNIVERSITÉ DU LUXEMBOURG
SNT

1.

Visual Studio Code



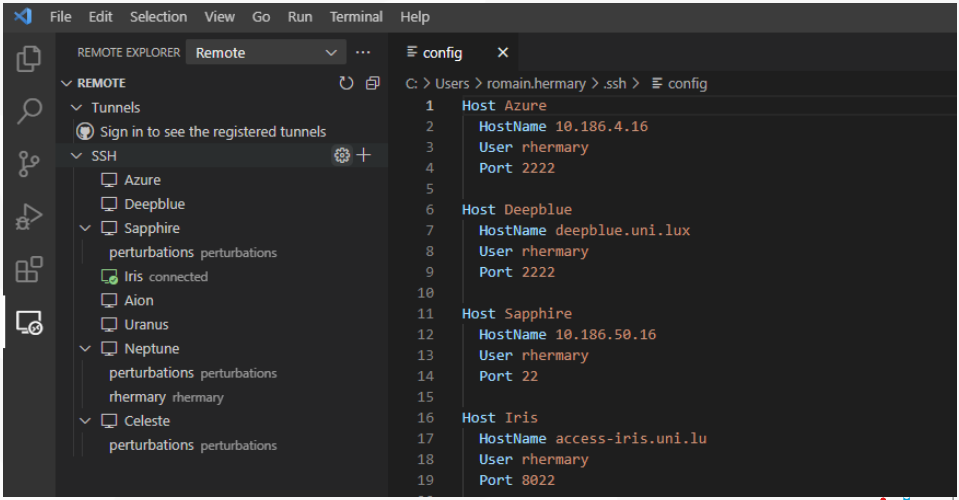
What Do I Use It For?

Everything

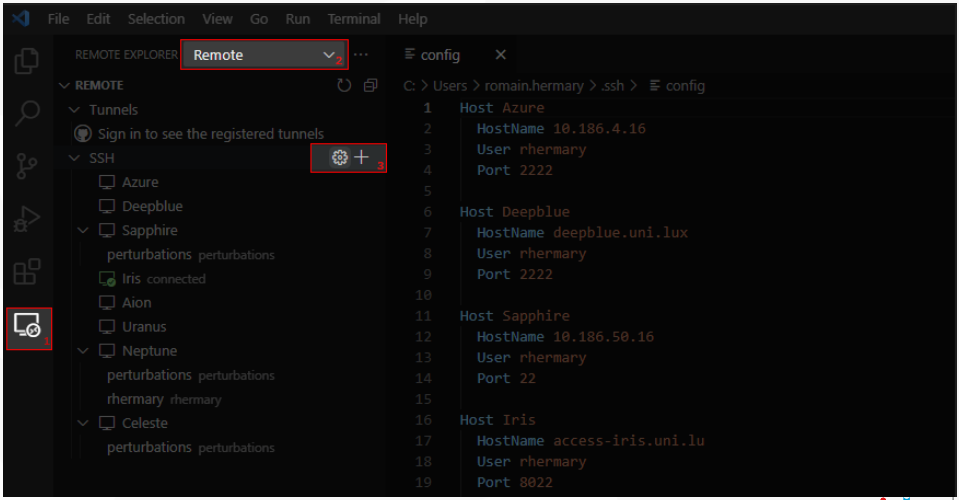
- Connect to a remote computer/server (and **WSL** on **Windows**)
- Open multiple terminals on the remote
- Automatize environment launching (can be different for each projects)
- Intuitive built-in debugger
- Efficient use of version control systems (**Git**)
- Very fast code navigation
- Awesome extensions
- ...

Note: **VSCode** is actually a nice text editor, not an *IDE*, ideal for development, debugging, etc.

SSH With VSCode



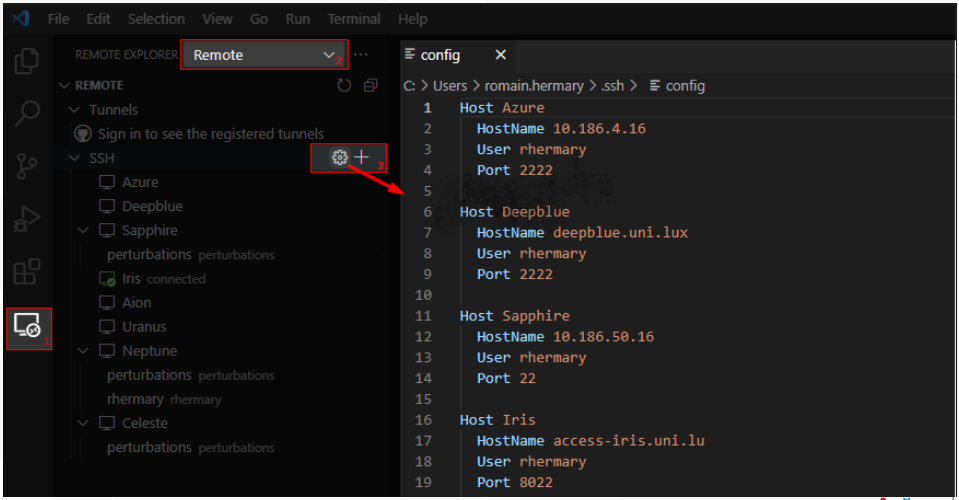
SSH With VSCode



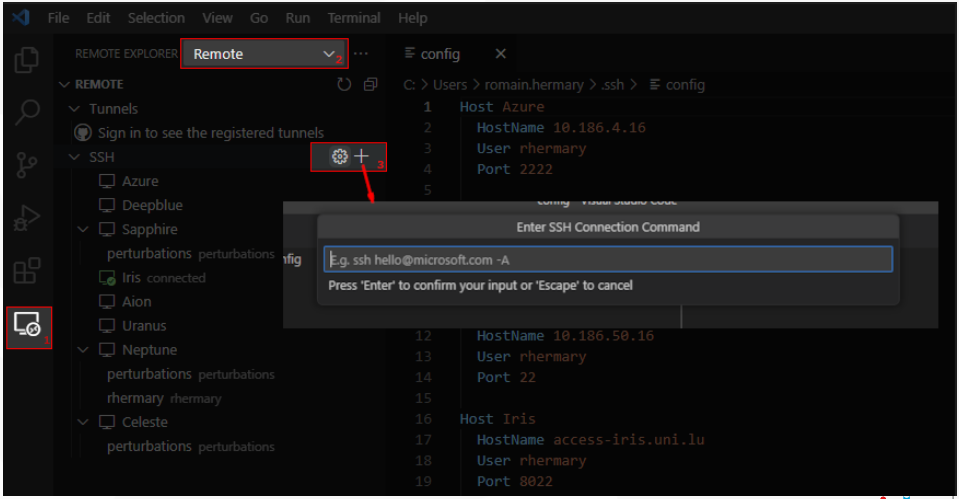
UNIVERSITÉ DU LUXEMBOURG

SnT

SSH With VSCode



SSH With VSCode



SSH With VSCode

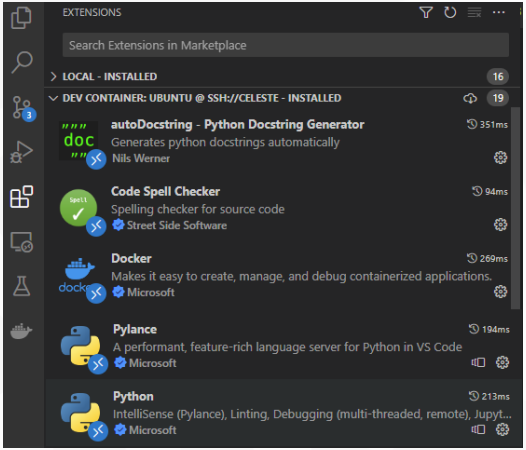
Tips:

- You might need to specify a private-key file or start an agent (more *here*)

```
Host name-of-ssh-host-here
  User your-user-name-on-host
  HostName host-fqdn-or-ip-goes-here
  IdentityFile ~/.ssh/id_ed25519
```

- I personally have:
  - A vault (with **1Password**), to manage/generate my keys – *and passwords!*
  - The extension for **VSCode** to automatically use and forward these keys

Market Place & Extensions

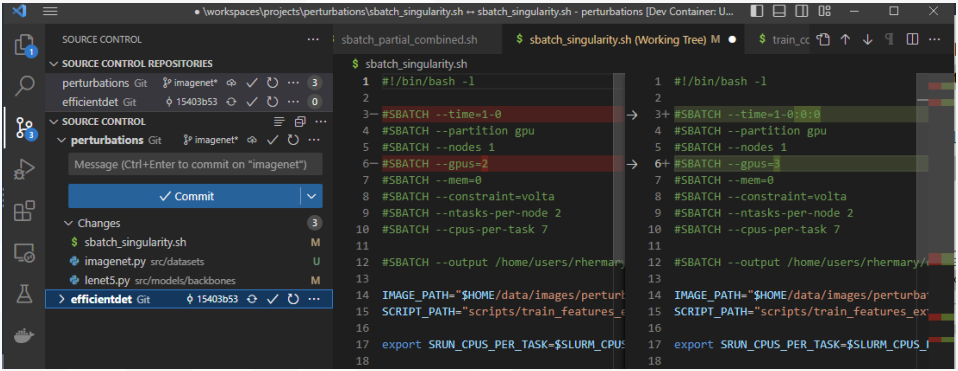


Find your happiness:

- Spell checker
- Language specific highlighting/helpers
- Visualization/preview tools
- Automating tools
- API bridges (Azure, SQL databases, Rest Client, etc.)
- Vim
- ...

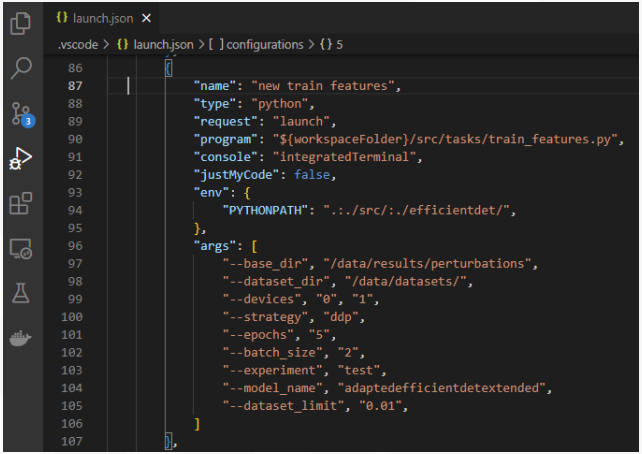
See all available extensions on the application or on the dedicated *web-page*

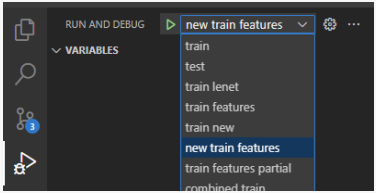
Git Without CLI



Disclaimer: Knowing how to use **Git** and other classic tools via the command line is still very important, do not rely solely on the GUI interface

The Debugger

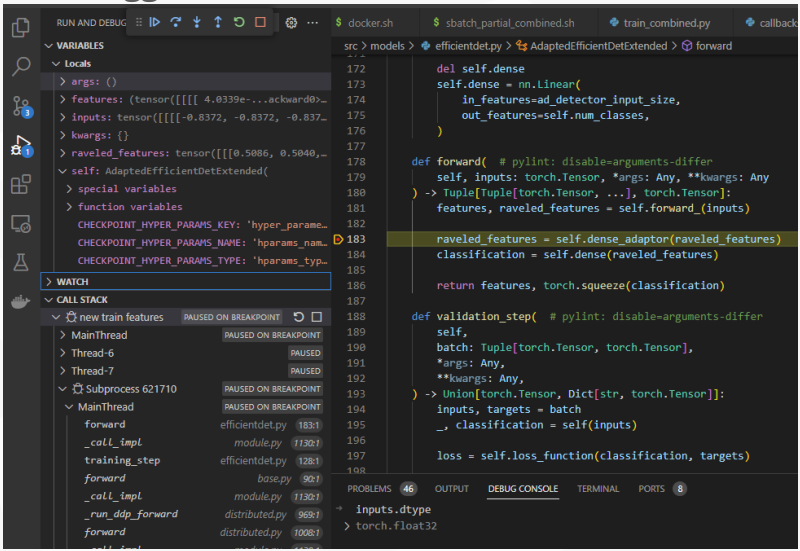




1. Go on the debug tab, and create a `lauch.json` file
2. Create a new command setting
3. Select the experiment and start the debug session

More debug tips on *this* page

The Debugger



- No more prints
- Stop where you want (`breakpoints`)
- Go backward in the call stack
- Test fixes
- View variables states
- Faster to use than `pdb` directly

UNIVERSITÉ DU LUXEMBOURG

Common Shortcuts

- `Ctrl` + `` ` `` : Open the terminal panel
- `Ctrl` + `Shift` + `P` : Open the command search bar (palette)
- `F5` : Launch the selected debug command (or relaunch the last one)
- `Ctrl` + `F5` : Launch the debug command without stopping at breakpoints
- `Ctrl` + `Left Click` : Go at the definition of the hovered object

Find more on the dedicated *web page*, or directly on **VSCode** by searching `Preferences: Open Keyboard Shortcuts` in the command palette

Useful Links

Specific Tutorials:

- **Python** Tips
- **Python** Environments
- **Jupyter** Notebooks debug mode

General Knowledge:

- *Complete documentation*
- Allowing breakpoints in external libraries (*disabling* `JustMyCode`)
- *Code Navigation*
- Use an `ssh-agent` and forward it (*avoid* creating a key/copypasting it on each server)
- **Intellisense**

NB: All the points above have clickable links!

2.
ULHPC

Infrastructures

Aion

- `access-aion.uni.lu`
- 354 CPU nodes
  - $256GB$ of **RAM** per node
  - 128 cores per node

Iris

- `access-iris.uni.lu`
- 24 GPU nodes ($756GB$ of ***RAM***, 28 cores)
  - 18 nodes with $16GB$ GPUs
  - 6 nodes with $32GB$ GPUs
- 172 CPU nodes
  - 168 with $168GB$ of **RAM** & 28 cores
  - 4 with $3072GB$ of **RAM** & 112 cores

Benefit from $500GB$ personal homes directories (backed-up), shared projects folder of multiple terabytes[1] (access the *same* files/folders via the two different servers).

- The full documentation on how to use the clusters: `https://hpc-docs.uni.lu/`
- Very complete tutorials from the university on *everything*: `https://ulhpc-tutorials.readthedocs.io/`

[1] `https://hpc-docs.uni.lu/data/layout/`

Resource Managment with SLURM

"Open source, fault-tolerant, and highly scalable cluster management and job scheduling system"[2]

- Software allowing resource management
- Interacting with this process is mandatory to access resources
- A resource request is called a *job*
- **SLURM** manages a queue of jobs, prioritise and schedule them

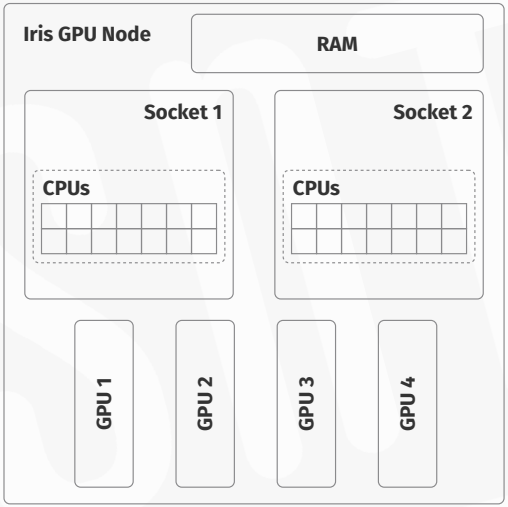
[2] `https://ulhpc-tutorials.readthedocs.io/en/latest/basic/scheduling/`

- More on **SLURM** on ULHPC in the *documentation*

Clusters


Cluster X
Partition 1
Node 1
Node 2
Node 3
Node N_{n1}
Partition N_p
Node 1
Node 2
Node 3
Node N_{n2}

Nodes Structure: An Example



When using a node, you can ask for a partial amount of the resources

- *e.g.* 14 CPUs, 2 GPUs and $100GB$ of RAM for 1 job

When demanding resources, try to ask for coherent amounts

- Use only what you need (beneficial for everyone)
- Adapt the number of threads and the settings to match the physical characteristics of the nodes[a]

[a] You can have a look at **NUMA** characteristics

Basic Commands

- `si` , `si-gpu`

  Custom commands which start an interactive session (allocate resource and attach your terminal to a node)[3]

- `srun`

  Used to submit a job for execution or initiate job steps in real time.

  - `$ srun -p <partition> -c <nb_cpus> -G <nb_gpus> <command>`

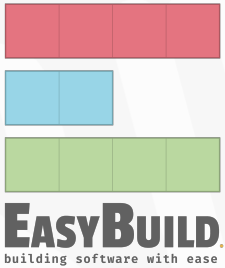
- `sbatch`

  Used to submit a job script for later execution. The script will typically contain one or more srun commands to launch parallel tasks..

  - `$ sbatch <script_file>.sh`

[3] More on interactive jobs *here*
More on the command options *here*

EasyBuild



"EasyBuild is a software build and installation framework that allows you to manage software on HPC systems in an efficient way."

- Apps/packages are available as loadable modules
- A good amount of software is already available on servers
- You can build your own modules or request them
- ***Spack*** *is an alternative*

- All already available modules: `https://hpc-docs.uni.lu/`
- Full **EasyBuild** documentation: `https://docs.easybuild.io/`

Interactive Example

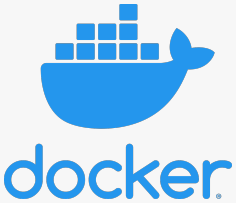
```
130 [rhermary@access1 ~]$ si -c 3
# salloc -p interactive --qos debug -C batch  -c 3
salloc: Pending job allocation 3151873
salloc: job 3151873 queued and waiting for resources
salloc: job 3151873 has been allocated resources
salloc: Granted job allocation 3151873
salloc: Waiting for resource configuration
salloc: Nodes iris-109 are ready for job
0 [rhermary@iris-109 ~](3151873 1N/T/1CN)$ module load lang/Python/3.8.6
0 [rhermary@iris-109 ~](3151873 1N/T/1CN)$ python --version
Python 3.8.6
0 [rhermary@iris-109 ~](3151873 1N/T/1CN)$ srun -n 3 python -c 'print("Hi, CVI2!")'
Hi, CVI2!
Hi, CVI2!
Hi, CVI2!
0 [rhermary@iris-109 ~](3151873 1N/T/1CN)$
```

Sbatch Script Example

```
#!/bin/bash -l

#SBATCH -N 2
#SBATCH --ntasks-per-node=1
#SBATCH -c 1
#SBATCH --time=0-00:05:00
#SBATCH -p batch

module purge
module load lang/Python

srun -n ${SLURM_NTASKS} python -c 'print("Hello World!")'
```

3.

Docker



What is Docker?

"Docker is an open source platform that enables developers to build deploy, run, update and manage containers"[4]

- **Docker** packages software into standardized units that have everything the software needs to run (including libraries, system tools, code, and runtime)
- It provides a standard way of running your code
- It allows to quickly deploy and scale applications into any environment and know your code will run

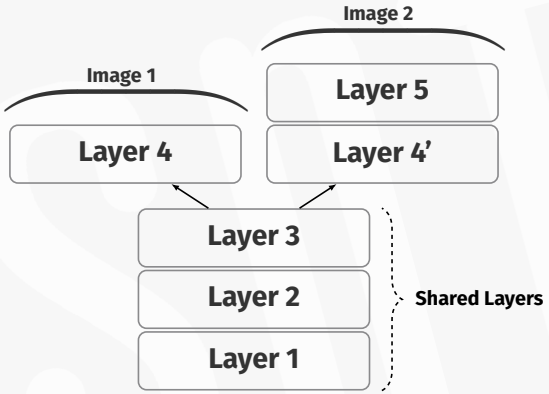
[4] `ibm.com`

Using Docker

1. Describe your environment in a `Dockerfile`
2. Construct your **Docker** image – `$ docker build ...`
3. Launch a process with the image as a template – `$ docker run ...`

Images Sources: `iconpacks.net`, `pngwing.com`, `onlinewebfonts.com`

Some More About Images



Why are they cool?

- A layer is equivalent to a change recorded on the base image/files
- Sharing layers allows
  - Faster image building
  - Lower memory impact
- Images are not copied when launching a container![5]

[5] Rather, a *copy-on-write* layer is *created* – copy happens only when a change on shared data happens.

Why Docker? *(In Short)*

Mainly, consistency

- A more complete and stable environment than **Conda**
- Having the same environment everywhere (on different servers, different computers…)
- Sharing the environment with others (easy configuration sharing when working in teams, ship it with your article)

But also

- Possibility to modify your code while your are running experiments inside a container – *a downside of interpreted languages*
- One image for multiple users reduces the memory footprint
- `root` permissions[6], not to depend only on preinstalled packages

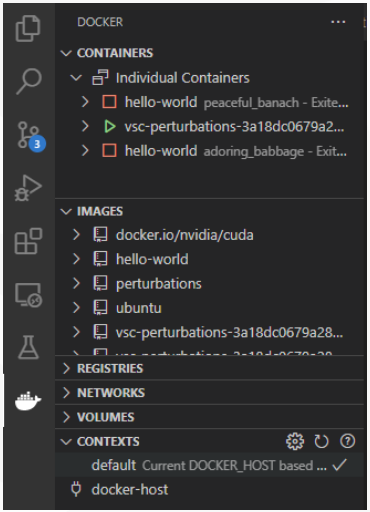
[6] Careful, use them *wisely*

Good Practices

- **Tag** or **label** your images with your name
- Try to **organize** *optimally*[7][8] your building steps
  - Minimize the number of layers
  - While maximizing the number of shareable layers between different images
- Containers should be
  - Stopped when not using it
  - Removed when stopped[9]
- **Nothing** should be stored in the containers (use mount points)

[7] Some advice in *this* post
[8] More best practices for writing your `Dockerfile` in the *documentation*
[9] I would make an exception for *DevContainers*

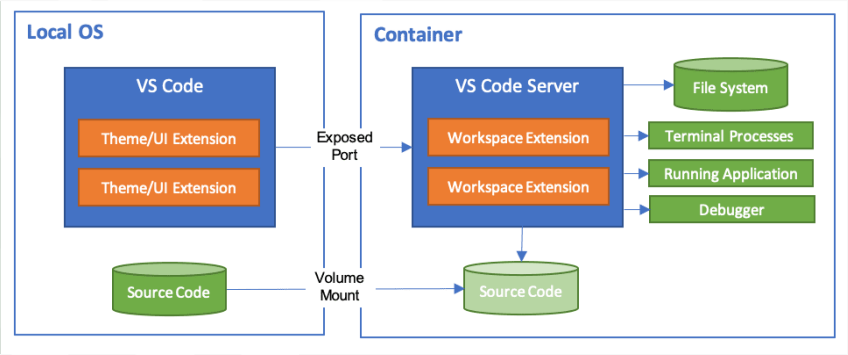
Combining Docker & VSCode



- **Docker** extension is available on **VSCode**
- Nicely visualize:
  - Containers (and their states)
  - List locally available images
  - List available volumes, networks, contexts, registries...
  - *Build, deploy*

Combining Docker & VSCode: Dev Containers

What about developing inside a container?



Source: code.visualstudio.com

The extension is from **Microsoft**, and can be found in the *marketplace*

Using the Dev Containers

Automatic configuration setup

```
/project-folder
├── .devcontainer
│      └── devcontainer.json
└── [...]  # Your project files
```

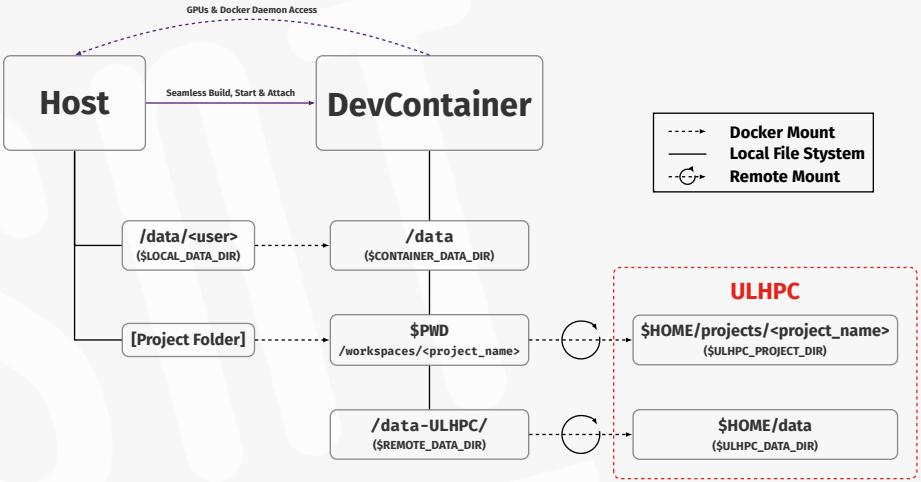
- Only adding a folder with a configuration file
- When opening your project folder, **VSCode** will detect this folder; you just need to *reopen* it in a container

My custom approach

```
/git-repo
├── project-folder
│   └── .devcontainer
│         ├── devcontainer.json
│         ├── Dockerfile
│         ├── .env
│         ├── postCreateCommand.sh
│         └── postStartCommand.sh
└── another-project
    └── .devcontainer
          └── [...]
```

But, where are my project files?

Combining Docker, VSCode & ULHPC Services



Find the template here: `https://gitlab.uni.lu/rhermary/workflow-template`

4.

Singularity

Yet Another Container Runtime

"Designed for ease-of-use on shared multi-user systems and in HPC environments"[10]

- Designed to be simple, fast, and secure
- Little memory/CPU overhead
- Fast instantiation and tear-down
- Compatible with **Docker** images
- Root elevation is needed for building
- Images are immutable, you can write only on mounted folders
- Default mounts: `$HOME` , `/tmp` , `/proc` , `/sys` , `/dev` , `$PWD`

[10] `https://hpc.auburn.edu/hpc/docs/hpcdocs/build/html/easley/containers.html`
Tutorial: `https://ulhpc-tutorials.readthedocs.io/en/latest/containers/singularity/`
Official Webpage: `https://sylabs.io/singularity/`

Some Commands

Build an image from a definition file

```
$ sudo singularity build image.sif Singularity.def
```

Pull and exec a command in a container

```
$ singularity pull docker://python:3.8.0b1-alpine3.9
$ singularity exec python_3.8.0b1-alpine3.9.sif python3
$ singularity shell python_3.8.0b1-alpine3.9.sif
```

Build an image from a compressed Docker image

```
$ sudo singularity build <image_name>.sif docker-archive://<archive_name>.tar
```

Run with GPU accessibility `$ singularity run --nv image.sif`

Load Singularity module `$ module load tools/Singularity`

5.

Miscellaneous

Libraries

- ***PyTorch Lightning*** – ***PyTorch*** *research framework*
  - Website – `https://www.pytorchlightning.ai/`
  - Documentation – `https://lightning.ai/docs/...`
  - Source Code – `https://github.com/Lightning-AI/...`
  - Colab Example – `https://colab.research.google.com/...`

NB: The displayed links might be shortened; click on them!

Libraries: Pytorch Lightning (Module)

```python
class LitAutoEncoder(pl.LightningModule):
    def __init__(self, encoder, decoder):
        super().__init__()
        self.encoder = encoder
        self.decoder = decoder

    def training_step(self, batch, batch_idx):
        # training_step defines the train loop.
        x, y = batch
        x = x.view(x.size(0), -1)
        z = self.encoder(x)
        x_hat = self.decoder(z)
        loss = F.mse_loss(x_hat, x)
        return loss

    def configure_optimizers(self):
        optimizer = torch.optim.Adam(self.parameters(), lr=1e-3)
        return optimizer
```

Source: lightning.ai

Libraries: Pytorch Lightning (DataModule)

```python
class MNISTDataModule(pl.LightningDataModule):
    def __init__(self, data_dir: str = "path/to/dir", batch_size: int = 32):
        super().__init__()
        self.data_dir = data_dir
        self.batch_size = batch_size

    def setup(self, stage: str):
        self.mnist_test = MNIST(self.data_dir, train=False)
        self.mnist_predict = MNIST(self.data_dir, train=False)
        mnist_full = MNIST(self.data_dir, train=True)
        self.mnist_train, self.mnist_val = random_split(mnist_full, [55000, 5000])

    def train_dataloader(self):
        return DataLoader(self.mnist_train, batch_size=self.batch_size)

    def val_dataloader(self):
        return DataLoader(self.mnist_val, batch_size=self.batch_size)

    def test_dataloader(self):
        return DataLoader(self.mnist_test, batch_size=self.batch_size)
```

Source: lightning.ai

Libraries: Pytorch Lightning (Trainer)

```
# model
autoencoder = LitAutoEncoder(Encoder(), Decoder())

# train model
trainer = pl.Trainer()
trainer.fit(model=autoencoder, train_dataloaders=train_loader)
```

Source: lightning.ai

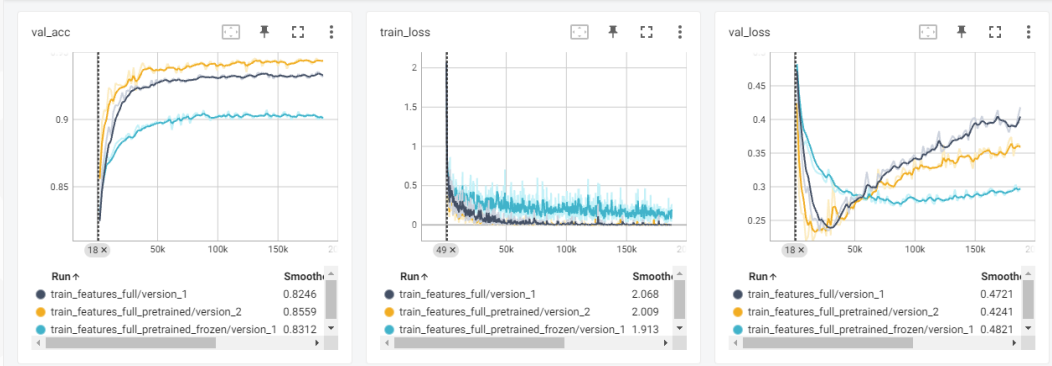
Libraries

- ***Black*** – ***Python*** *code formatter*
  - PyPi – `https://pypi.org/project/black/`
  - Documentation – `https://black.readthedocs.io/`
- ***MyPy*** – ***Python*** *static type checker*
  - PyPi – `https://pypi.org/project/mypy/`
  - Documentation – `https://mypy.readthedocs.io/`
  - Also read about typing – `https://docs.python.org/...`
- ***PyLint*** – ***Python*** *static code analyser*
  - PyPi – `https://pypi.org/project/pylint/`
  - Documentation – `https://pylint.readthedocs.io/`

Libraries

- ***TensorBoard*** – *Tracking and visualizing metrics*
  - Website – `https://www.tensorflow.org/tensorboard`
  - Guide – `https://www.tensorflow.org/tensorboard/get_started`
  - PyTorch Profiler – `https://pypi.org/project/torch-tb-profiler/`
- ***MLFlow*** – *Tracking ML experiments*
  - Website – `https://mlflow.org/`
  - Documentation – `https://mlflow.org/docs/`

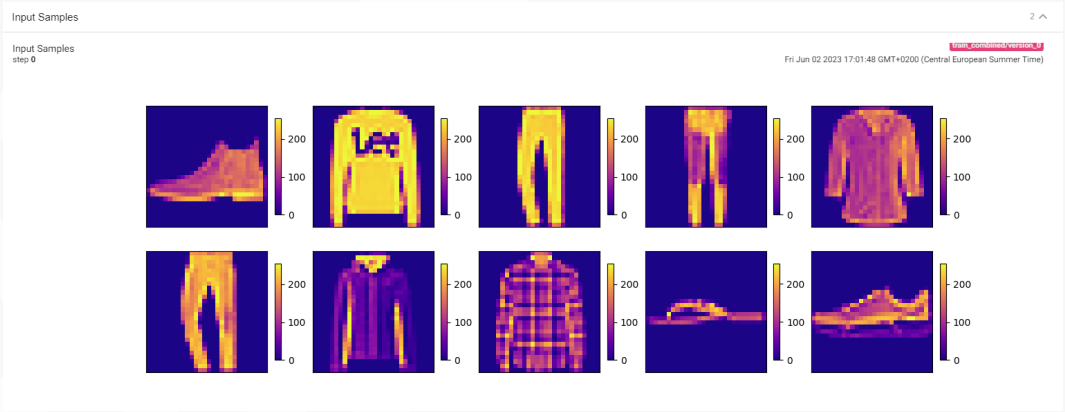
Libraries: Tensorboard (Charts)



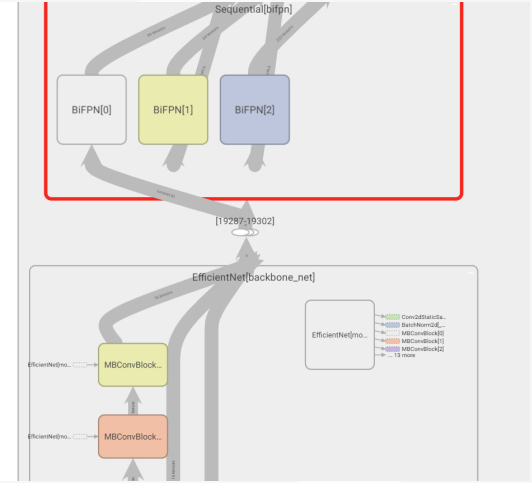
UNIVERSITÉ DU LUXEMBOURG

SnT

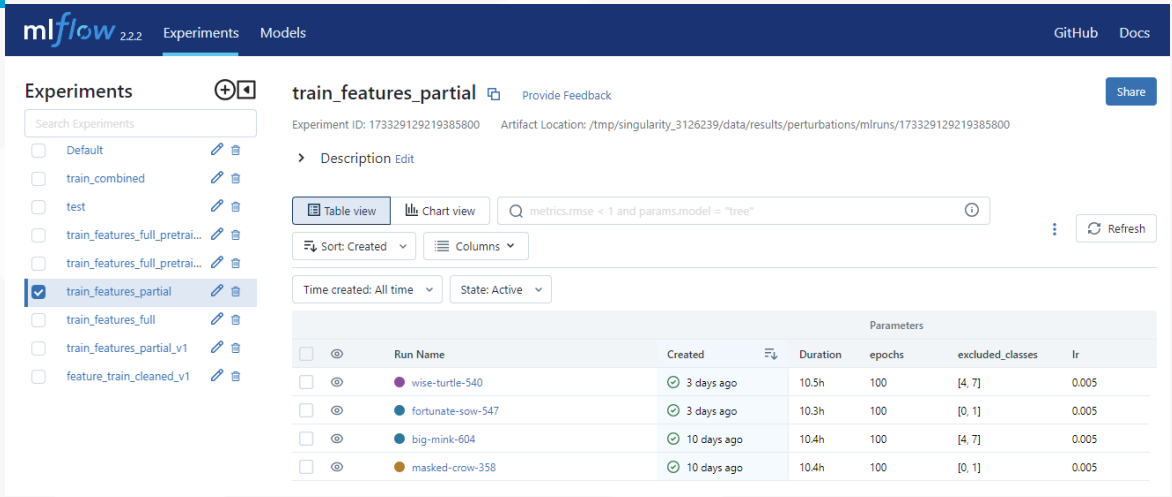
Libraries: Tensorboard (Images)



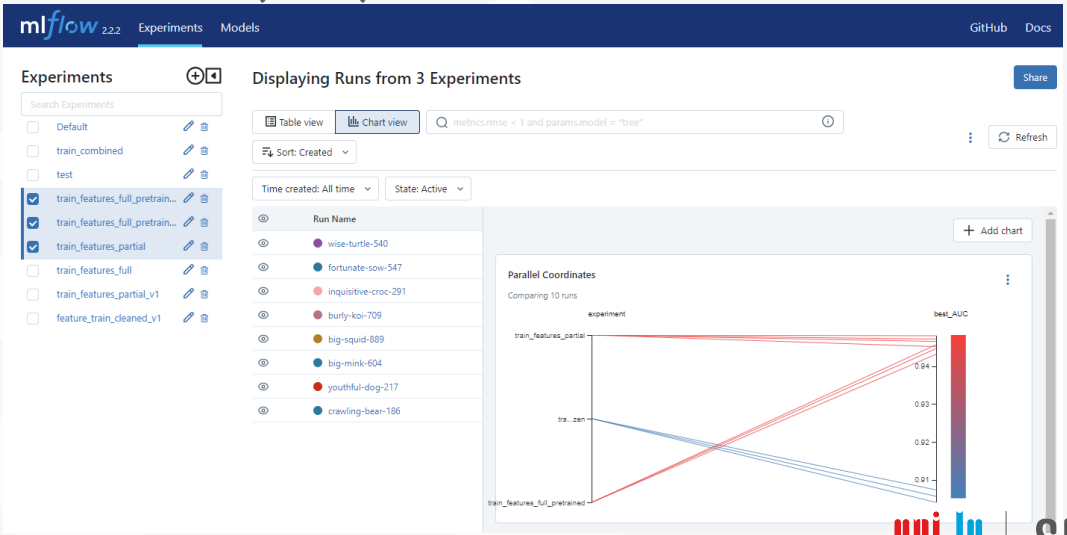
Libraries: Tensorboard (Graphs)



Libraries: MLFlow (Experiments Table)



Libraries: MLFlow (Charts)



Other Tips

- **ULHPC** *tutorials* website has a huge amount of resources
  - SSH, CUDA, deep learning, SLURM, Python, Singularity...
- Use **Version Control Systems (VCS)** – ***Git***
  - Push *before* running your experiments
  - Run your code on a specific commit, not on modified files
- Do not rush your experiments; running does not mean working
- **Jupyter** notebooks are handy for quick data analysis, but use **Python** scripts when running experiments[11]
- Start using ***Object Oriented Programming (OOP)***

[11] Some reasons why in *this* article

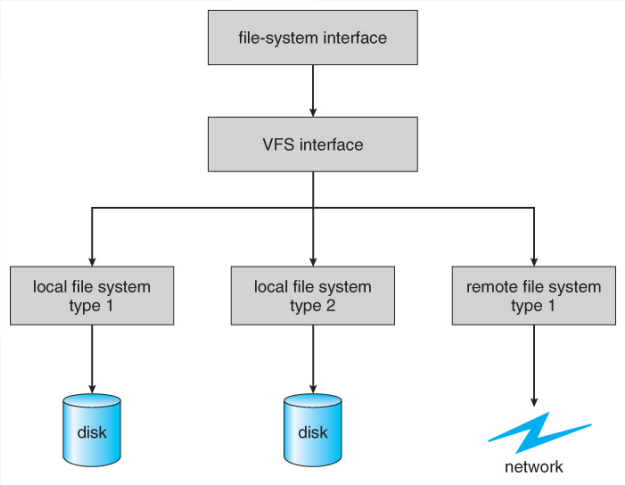
Other Tips

- Use LaTeX – `https://www.latex-project.org/`
  - ***Beamer*** – `https://en.wikipedia.org/wiki/`
  - Template – `https://gitlab.uni.lu/rhermary/snt-beamer-template`
- ***RTFM***
- Lock your computer (and turn it off)
  - ⊞ + L
  - Ctrl + ⌘ + Q
  - 🐧 + L or Ctrl + Alt + L
  - Instead of letting your computer run unlocked for some random task, look at `tmux` (terminal multiplexer)

Thanks for your attention!

Questions?

Directory Mounting (File System Functioning)



Source: `cs.uic.edu`

Dockerfile: Example

```
FROM ubuntu:20.04
LABEL maintainer="rhermary"

WORKDIR /app/
COPY requirements.txt requirements.txt
ENV PYTHONPATH src:efficientdet

ENV DEBIAN_FRONTEND noninteractive
RUN apt-get update -y\
   && apt-get install curl wget software-properties-common build-essential git -y\
   && add-apt-repository ppa:deadsnakes/ppa -y\
   && apt install python3.10 python3.10-distutils -y\
   && update-alternatives --install /usr/bin/python python /usr/bin/python3.10 1\
   && curl -sS https://bootstrap.pypa.io/get-pip.py | python\
   && python -m pip install --upgrade pip

RUN python -m pip install -r requirements.txt
CMD /bin/bash
```

Obsidian

Model

- Very light-weight
- lenet-5 classifier
- VAE as a noise generator (perturbator)

XP Details

-

Error Function

From my understanding, they use VAEs because they needed a generative model to produce the noises, and because of the loss function which permits them to add some restrictions on the noise easily.

Annotations

is usually a unsupervised learning task

> *Page 1*

maps the data into high-dimensional feature space

> *Page 1*

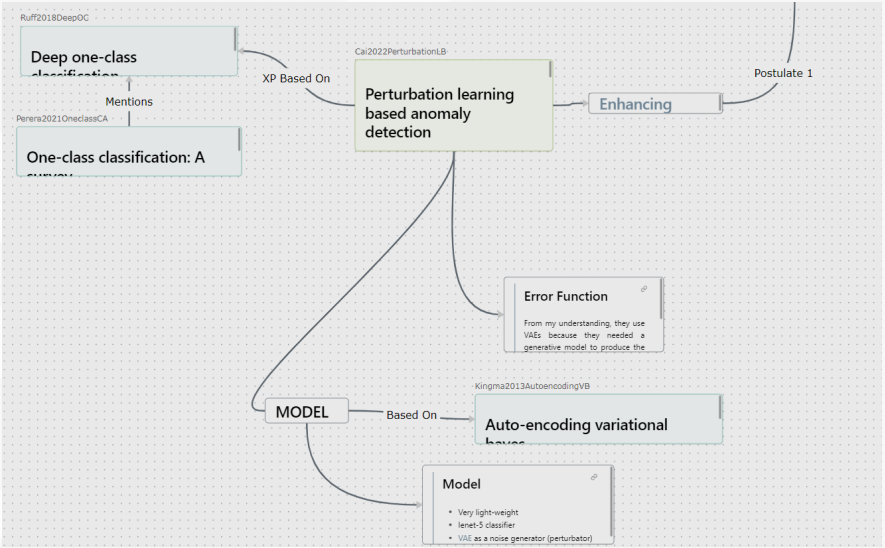
ot suitable for large-scale data due to the high computational cost

> *Page 1*

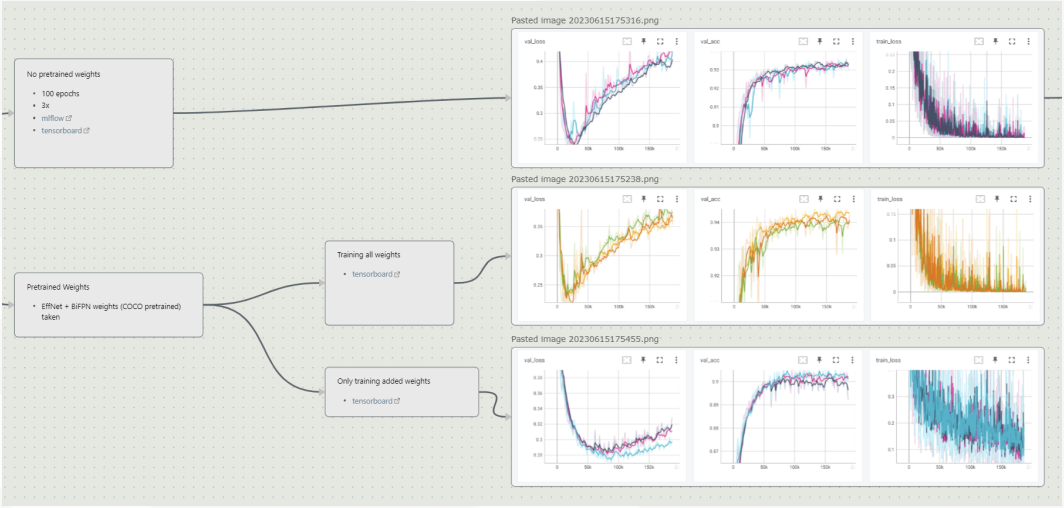
Instead, they usually use the data reconstruction error as a metric to detect anomalies

> *Page 1*

Obsidian


Ruff2018DeepOC
Deep one-class
XP Based On
Cai2022PerturbationLB
Perturbation learning based anomaly detection
Postulate 1
Enhancing
Mentions
Perera2021OneclassCA
One-class classification: A
Error Function
From my understanding, they use VAEs because they needed a generative model to produce the
Kingma2013AutoencodingVB
MODEL
Based On
Auto-encoding variational
Model
Very light-weight
lenet-5 classifier
VAE as a noise generator (perturbator)

Obsidian


No pretrained weights
100 epochs
3x
mlflow
tensorboard
Pretrained Weights
EffNet + BiFPN weights (COCO pretrained) taken
Training all weights
tensorboard
Only training added weights
tensorboard
Pasted image 20230615175316.png
Pasted image 20230615175238.png
Pasted image 20230615175455.png
val_loss
val_acc
train_loss