晶創25 (Nano 5)

- 2025/06
- 計算力 13.06 PFLOPS
- Top500 # 118
- Green500 # 72

How to use Nano5 of NCHC?

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Outline

- Introduction
- Login to Nano5 server
- Train an image classification model
- Slurm file explanations
- Conclusions

1. Introduction

- Nano5: The latest supercomputer of NCHC released in 2025/4.
- Support H100/H200 GPUs, multi-core CPU, RAM, and HFS.
- H100 has the TF32 (989 TFLOPS) and BF16
- Nano5 runs the container of Singularity Image Format (SIF).
- nVIDIA NGC container could be directly employed.

GPU Spec	VRAM	# of GPUs on Nano5
H100	80 GB HBM3	168
H200	141 GB HBM3e	128

1. Introduction

- **Hourly Pricing and performance**

NCHC Platform	GPU Spec	FP32	TF32	FP16/BF16	NSTC	Academic
Nano5	H100 80GB	67 TFLOPS	989 TFLOPS	1979 TFLOPS	$25	$50
Nano5	H200 141GB	67 TFLOPS	989 TFLOPS	1979 TFLOPS	$30	$60
TWCC	V100 32 GB	15.7 TFLOPS	-	125 TFLOPS	$10	$20

- TF32 is on automatically without revising the code (e.g., loss scaling). Manually control of the TF32 is shown below.
- H100 has a better cost-performance ratio than V100 on TWCC (Taiwan Computing Cloud, or called TAIWANIA 2)

```
import torch
torch.backends.cuda.matmul.allow_tf32 = True
torch.backends.cudnn.allow_tf32 = True
```

1. Introduction

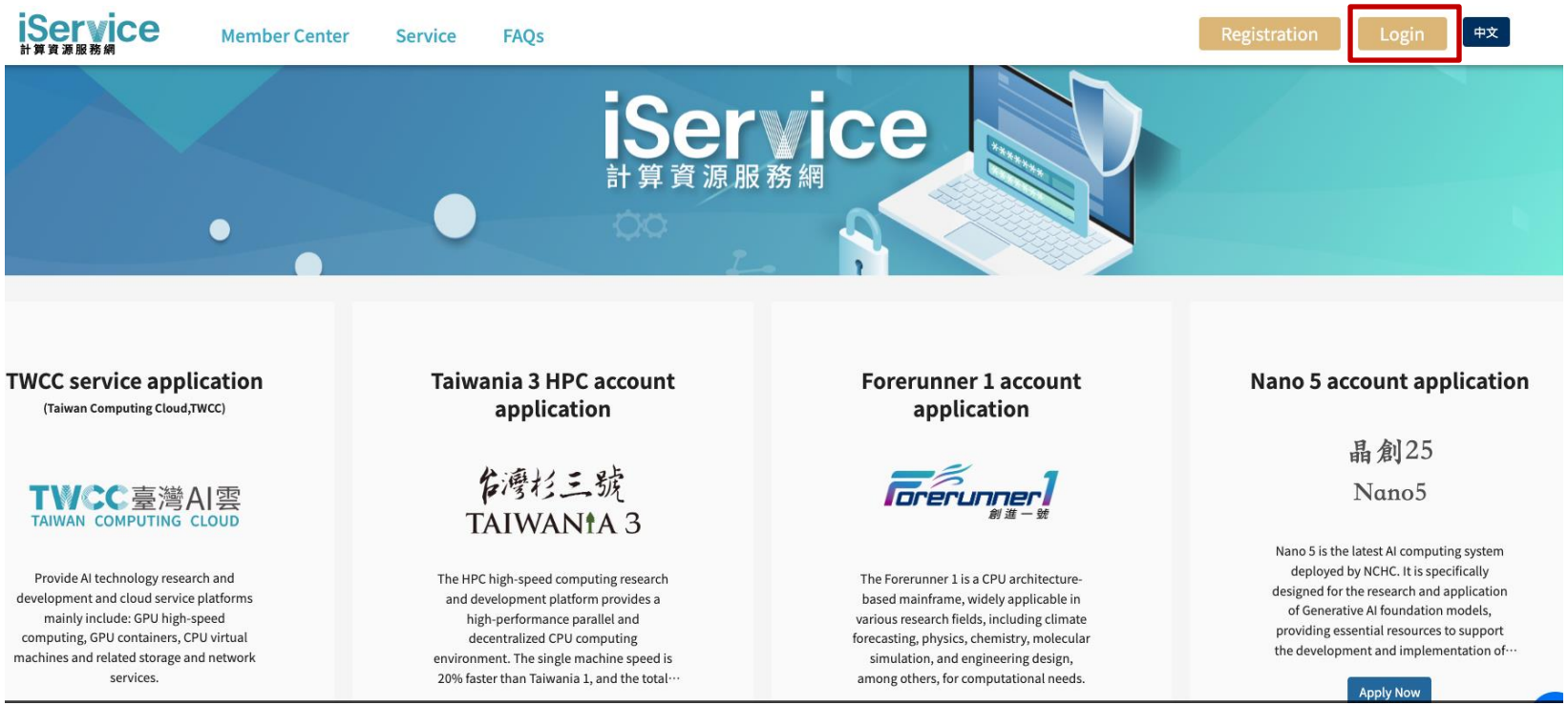
- NCHC uses Slurm (Simple Linux Utility for Resource Management) across the TWCC, TAIWANIA 3, Forerunner 1 (F1), and Nano5.
- Slurm is an open-source, highly scalable workload manager and job scheduler for Linux clusters that handles resource allocation, job queuing/scheduling, and accounting.
- Two important commands (srun and sbatch) is shown in the explanation of the Slurm file.

2. Login to Nano5 Server

- Three critical major topics here:
  - Set the server password
  - Connection by SSH client
  - Upload files/directories by FileZilla

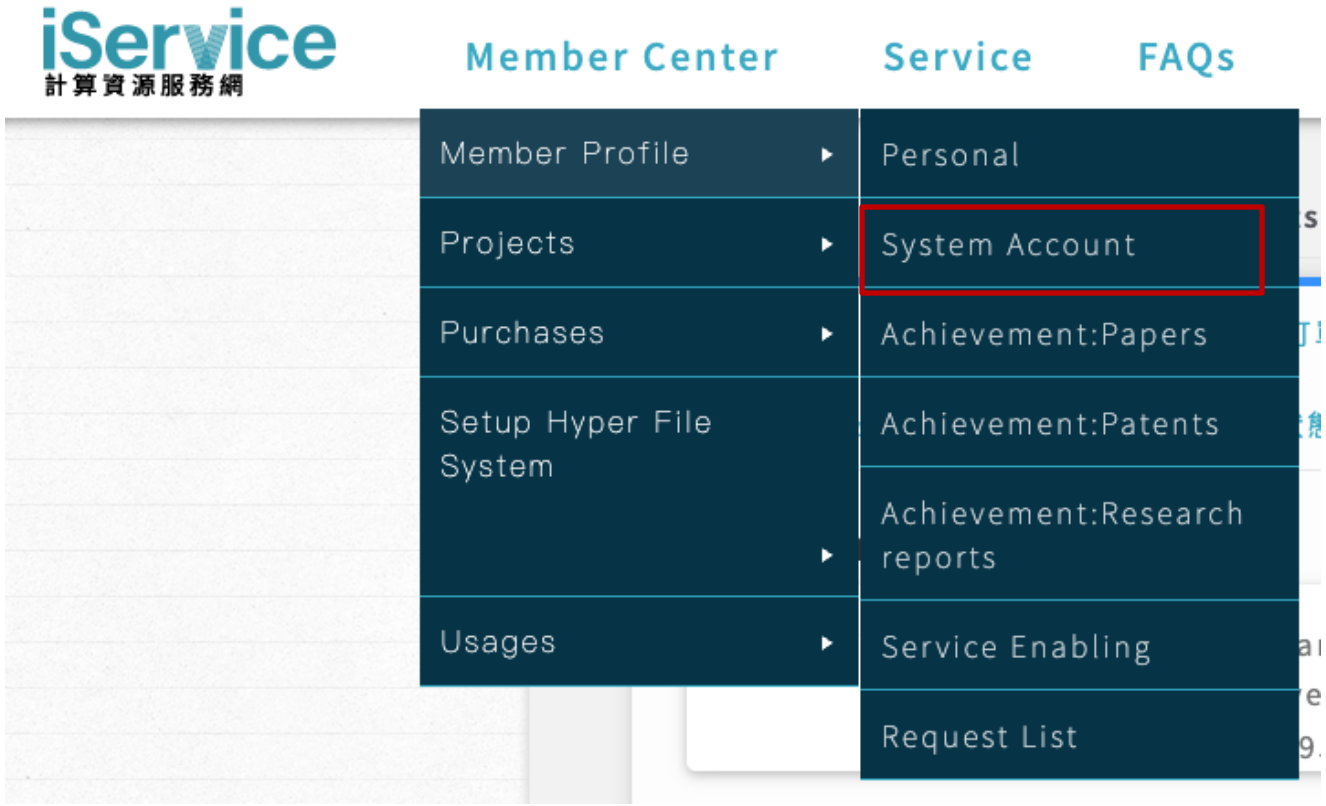
2.1 Set the server password

- Step 1: Login to HCHC Service Portal
- https://iservice.nchc.org.tw/nchc_service/index.php



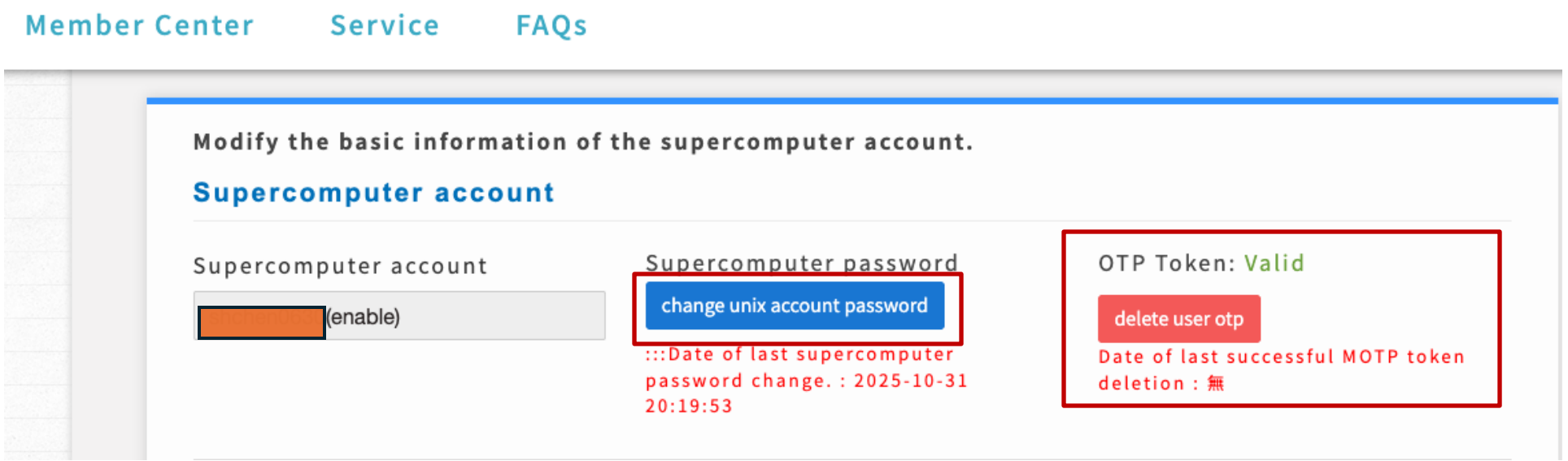
2.1 Set the server password

- Step 2: Select your project
- Step 3: Select Member Center/Member Profile/System Account



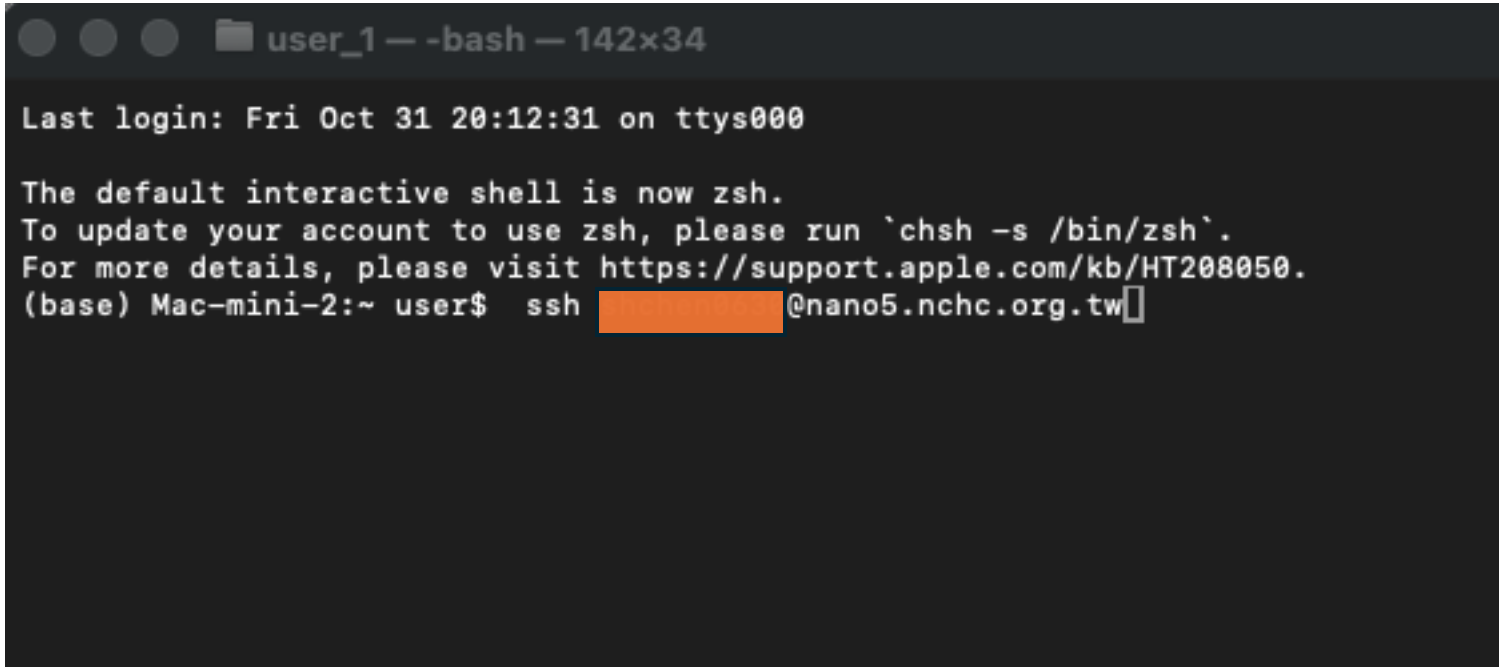
2.1 Set the server password

- Step 4: Record your account name (Orange area below)
- Step 5: Click “Change unix account password”
- Step 6 : Turn on the OTP. OTP by mobile App for faster 2-factor authentication



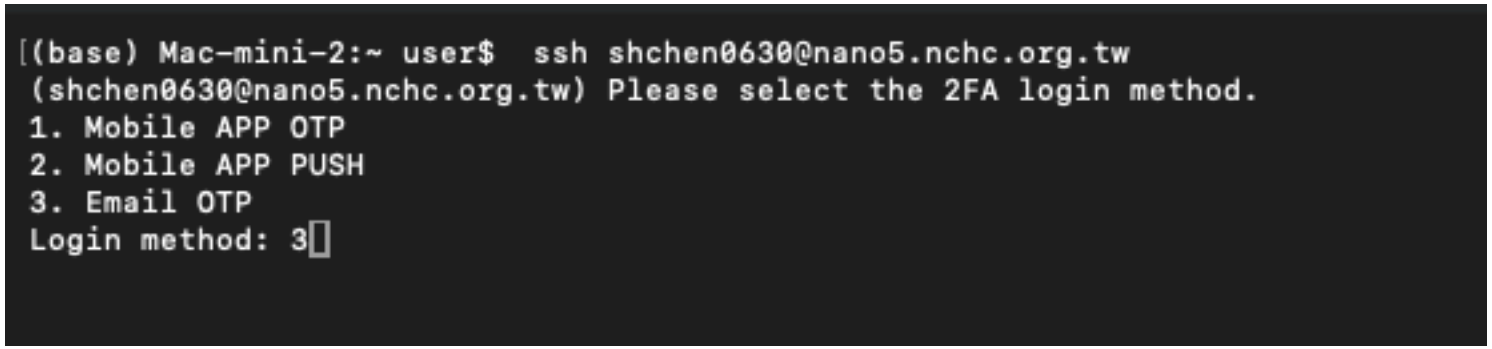
2.2 Connection by SSH client

- Step 1: We use the SSH to connect to the Nano5 Linux server
  - ssh *yourAccount*@nano5.nchc.org.tw
- If you use Windows, you could also use Putty.



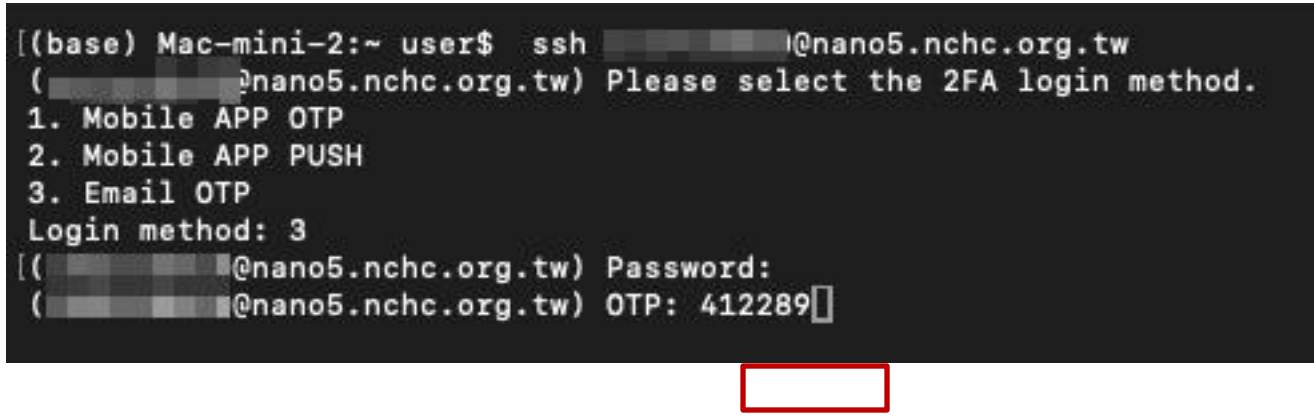
2.2 Connection by SSH client

- Step 2: Select a 2-factor login method. We use 3. Email OTP here.



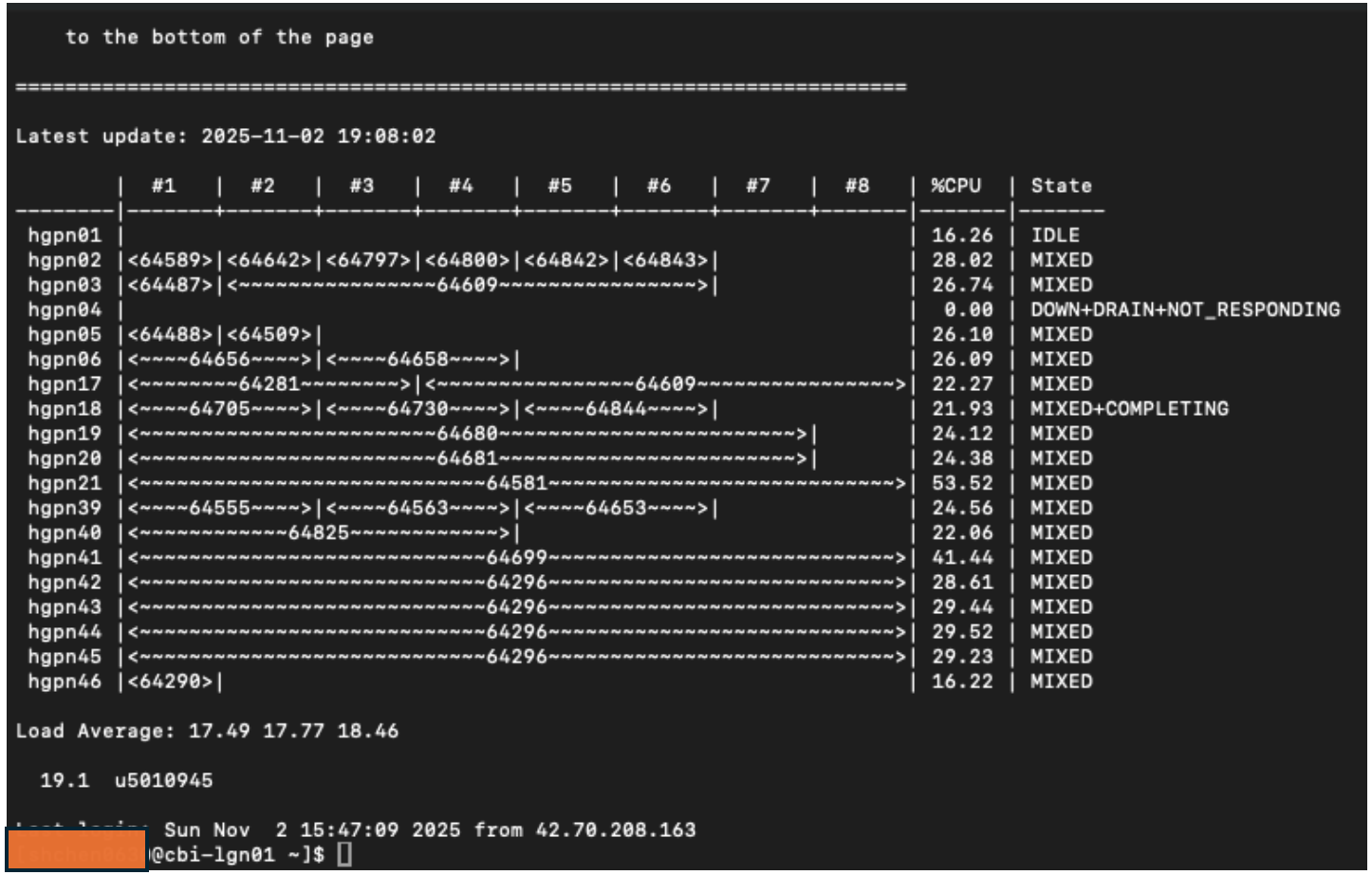
2.2 Connection by SSH client

- Step 3: Enter your password first and then check your email to obtain the OTP code.



2.2 Connection by SSH client

- Step 4: Login successfully!

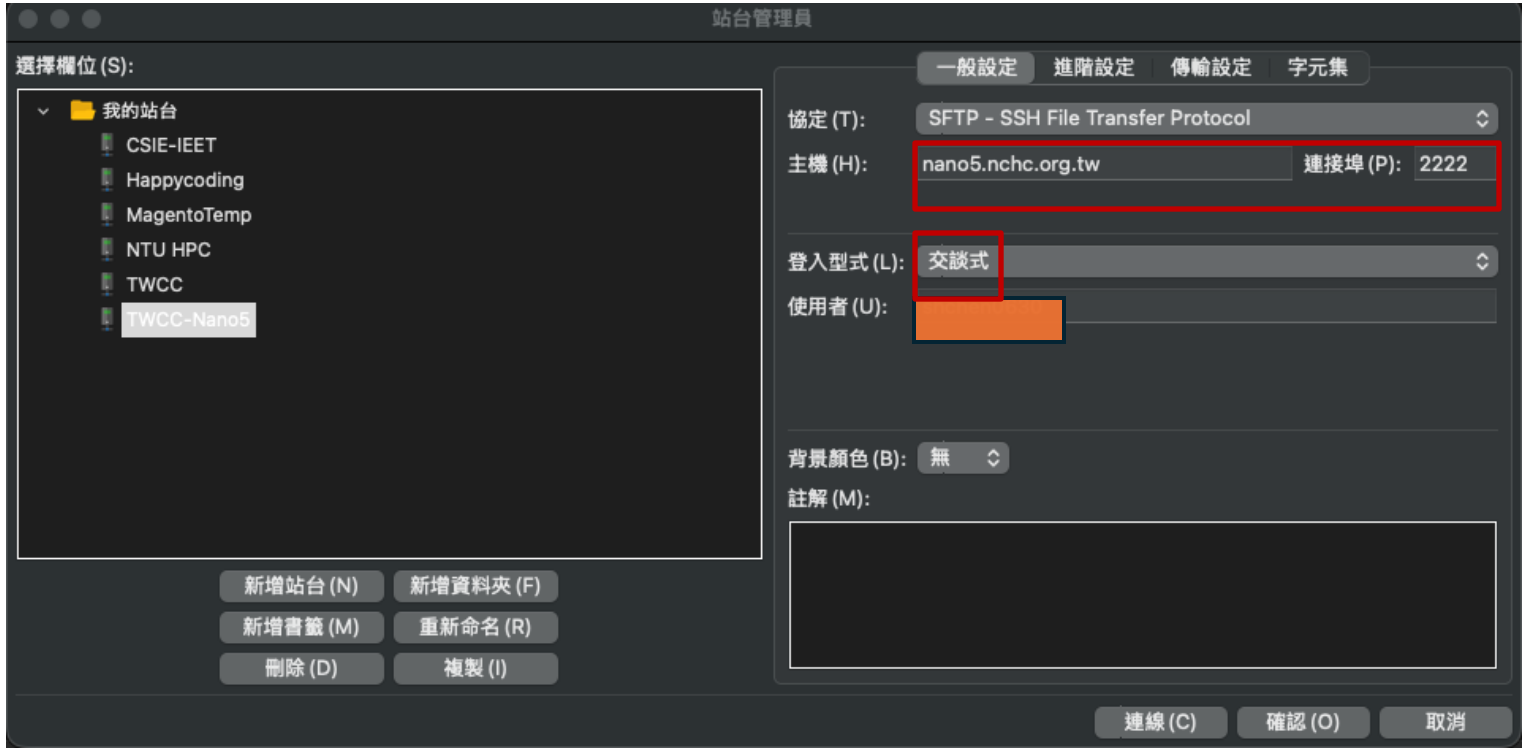


2.3 Upload files by FileZilla

- Step 1: Download the FileZilla (or WinSCP on Windows)
- Step 2: Create a new site. We use SFTP protocol from the dropdown menu.

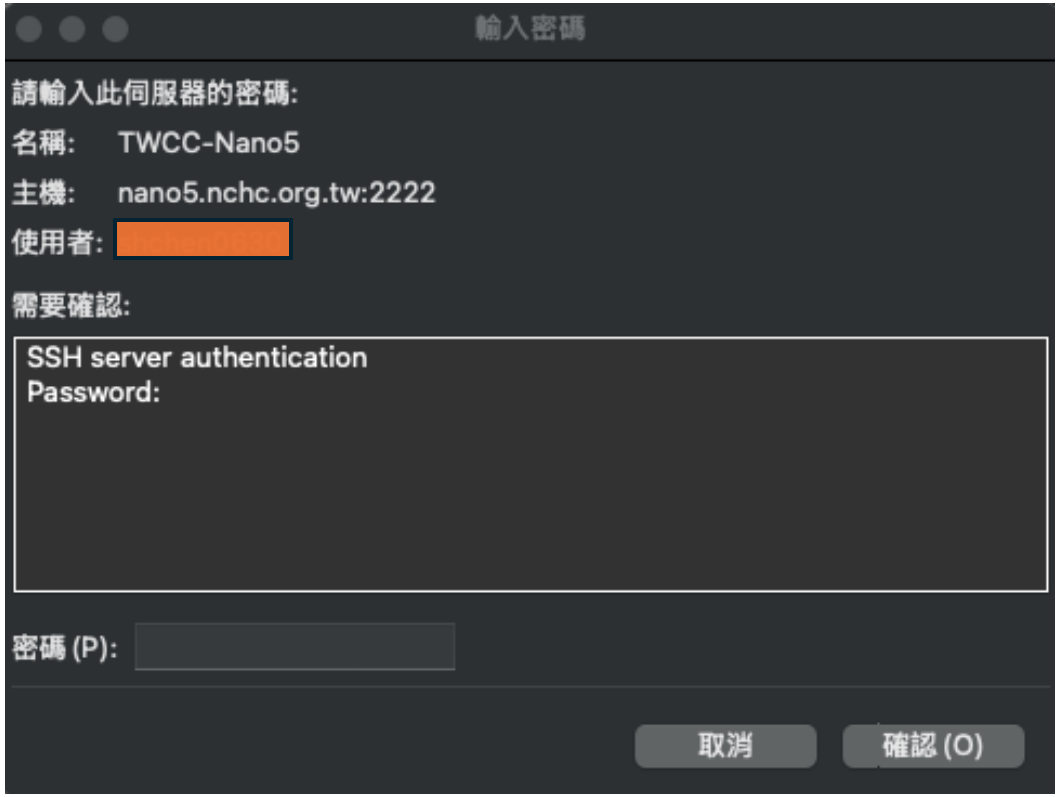
2.3 Upload files by FileZilla

- Step 3: Input Nano5 address (nano5.nchc.org.tw), port number 2222, *select the interactive login*, and your account.
- Interactive model will promote the login method, password, and code.



2.3 Upload files by FileZilla

- Step 3: After you click connect, there is a pop-up window. We input 3 (Email OTP) again. You input the password and OTP code.



2.3 Upload files by FileZilla

- Once it is connected, you could try to upload a file or a folder.
- The directory is under your HOME on the Nano5 Linux server.
- Extra: Try the Mobile App OTP method
  - After you make a successful connect to SFTP server, it is worthwhile to enable this method.
  - This method works more efficient.

3. Train an image classification model

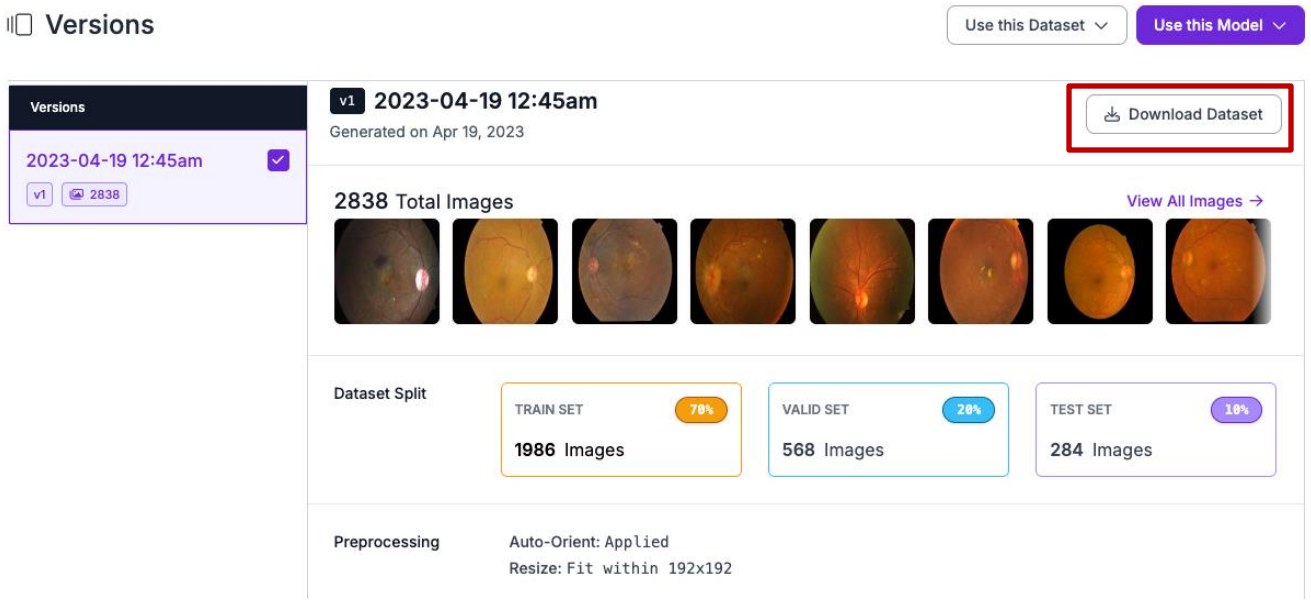
- We will upload the deep learning program and dataset.
- Besides, we write a Slurm script to deploy the training job(s).
- For simplicity, a demo project is provided.
- Please run git clone command the project on Nano5 :
  - git clone https://github.com/worldstar/NCHC-Slurm-Demo

3.1 Download a demo GitHub Project

- Credit of this all-in-one GitHub project
- **A. Image Classification Program:** timm (PyTorch Image Models)
  - https://github.com/huggingface/pytorch-image-models.git
  - A library of state-of-the-art PyTorch vision models (ResNet, EfficientNet, ConvNeXt, ViT, Swin Transformer） with pretrained weights plus training, inference, and evaluation utilities.
  - Maintained by Hugging Face now

3.1 Download a demo GitHub Project

- Credit of this all-in-one GitHub project
- **B. Dataset**
  - Diabetic Retinopathy Screening AI Computer Vision Model
  - https://universe.roboflow.com/ucla-master-of-quantitative-economics/diabetic-retinopathy-screening-ai



3.2 Revise the Slurm file

- Please edit the singularityClassification.slurm by text editor (vi or vim)
- Modify the account name is your project ID, starting with MSTXXXX or ACDXXXX.
- We explain the parameters. But please note the log files are with .out and .err sub filename.
- %x is job-name (cls-sing)
- %j is the job ID

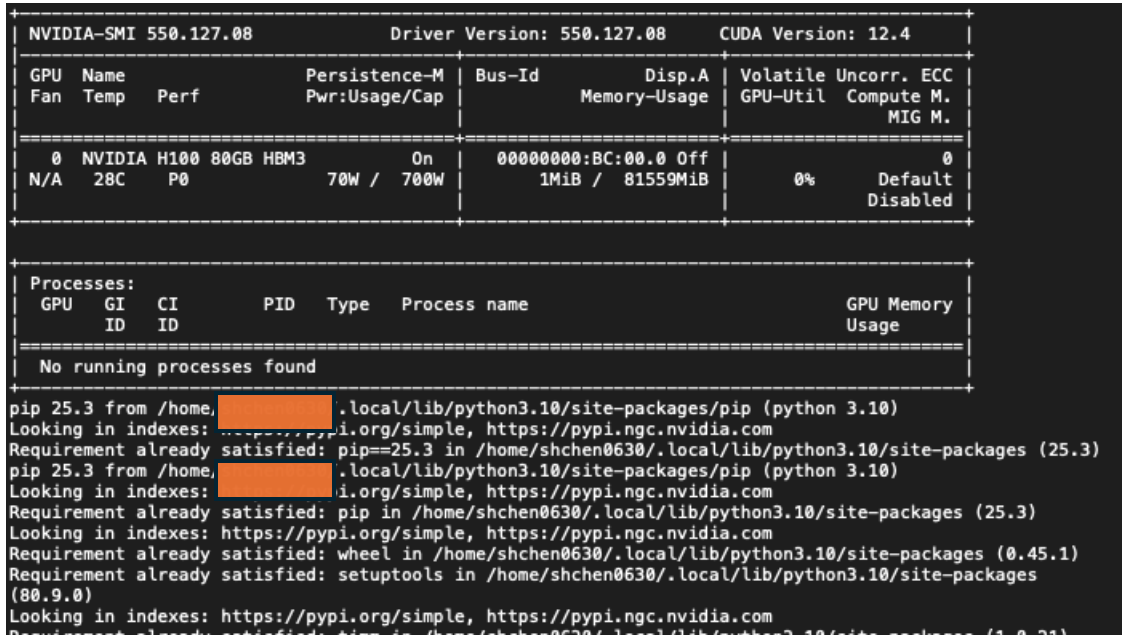
```
#!/bin/bash
#SBATCH --job-name=cls-sing
#SBATCH --partition=dev
#SBATCH --account=MSTXXXX     ## iService_ID 計畫 ID
## 選一種 GPU 申請方式（依叢集設定）
# 新版寫法（若支援）
##SBATCH --gpus=1
# 通用寫法（多數中心可用）
#SBATCH --gres=gpu:1
#SBATCH --cpus-per-task=8
#SBATCH --time=01:00:00
#SBATCH --output=%x-%j.out
#SBATCH --error=%x-%j.err
```

3.3 Run the Slurm file

- Step 1: Connect to the Nano5 by SSH.
- Step 2: Enter the project directory
  - cd ~/NCHC-Slurm-Demo/
- Step 3: Run the sbatch command
  - sbatch singularityClassification.slurm
- Step 4: You will read the job ID from the terminal

3.3 Run the Slurm file

- Step 5: Check your status of your batch job. It might be PD in the beginning; R is running.
  - squeue -u YOUR_ACCOUNT
- Step 6: Read the output log: cls-sing-XXXXX.out



3.4 Access Output Results

- Step 1: Read the error log: cls-sing-XXXXX.err under the same project folder

```
13:4: not a valid test operator: (
13:4: not a valid test operator: 550.127.08
Training with a single process on 1 device (cuda).
Model convnext_base created, param count:88591464
Data processing configuration for current model + dataset:
        input_size: (3, 512, 512)
        interpolation: bicubic
        mean: (0.485, 0.456, 0.406)
        std: (0.229, 0.224, 0.225)
        crop_pct: 0.875
        crop_mode: center
Created AdamW (adamw) optimizer: lr: 0.0005, betas: (0.9, 0.999), eps: 1e-08, weight_decay: 2e-05, amsgrad: False, foreach: None, maxi
False, differentiable: False, fused: None
Using native Torch AMP. Training in mixed precision.
Scheduled epochs: 50 (epochs + cooldown_epochs). Warmup within epochs when warmup_prefix=False. LR stepped per epoch.
Train: 0 [   0/31 (  3%)]  Loss: 7.10 (7.10)  Time: 22.751s,    2.81/s  (22.751s,    2.81/s)  LR: 1.000e-05  Data: 1.496 (1.496)
Test: [   0/8]  Time: 0.781 (0.781)  Loss:   4.566 ( 4.566)  Acc@1:   0.000 (  0.000)  Acc@5: 100.000 (100.000)
Test: [   8/8]  Time: 1.299 (0.300)  Loss:   7.317 ( 2.339)  Acc@1:   0.000 ( 50.528)  Acc@5:   0.000 ( 88.732)
Current checkpoints:
 ('./output/train/20251102-111549-convnext_base-512/checkpoint-0.pth.tar', 50.528169014084504)

Train: 1 [   0/31 (  3%)]  Loss: 4.15 (4.15)  Time: 0.961s,   66.62/s  (0.961s,   66.62/s)  LR: 1.080e-04  Data: 0.685 (0.685)
Test: [   0/8]  Time: 0.511 (0.511)  Loss:   2.922 ( 2.922)  Acc@1:   0.000 (  0.000)  Acc@5: 100.000 (100.000)
Test: [   8/8]  Time: 0.078 (0.152)  Loss:   3.780 ( 1.539)  Acc@1:   0.000 ( 50.704)  Acc@5:  96.429 ( 99.648)
Current checkpoints:
 ('./output/train/20251102-111549-convnext_base-512/checkpoint-1.pth.tar', 50.70422535211268)
 ('./output/train/20251102-111549-convnext_base-512/checkpoint-0.pth.tar', 50.528169014084504)
```

3.4 Access Output Results

- Step 2: Model Files and Summary.csv. Please go to ~/src/ NCHC-Slurm-Demo/output/train/XXX-convnext_base-512/

檔案名稱	檔案大小	檔案類型	最後修改時間	權限
..				
args.yaml	2,870	yaml-檔案	2025/11/02 11時15分49...	-rw-r--r--
checkpoint-33.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時22分4...	-rw-r--r--
checkpoint-36.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時23分17秒	-rw-r--r--
checkpoint-38.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時23分4...	-rw-r--r--
checkpoint-39.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時23分51...	-rw-r--r--
checkpoint-41.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時24分14...	-rw-r--r--
checkpoint-45.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時25分0...	-rw-r--r--
checkpoint-46.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時25分11秒	-rw-r--r--
checkpoint-47.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時25分2...	-rw-r--r--
checkpoint-48.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時25分3...	-rw-r--r--
checkpoint-49.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時25分4...	-rw-r--r--
last.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時25分4...	-rw-r--r--
model_best.pth.tar	1,063,524,714	tar-檔案	2025/11/02 11時23分51...	-rw-r--r--
summary.csv	4,992	csv-檔案	2025/11/02 11時25分4...	-rw-r--r--

epoch	train_loss	eval_loss	eval_top1	eval_top5	lr
29	9327575929	976230675062	1830985915	00000075219	0.00019
30	5652595796	800155286385	7394366197	10000075219	0.00017
31	6147473858	299669741241	0915492957	70000075219	0.00016
32	0147726151	3497153000	0915492957	70000075219	0.00014
33	6468450638	3223120461	7605633802	00000075219	0.00013
34	0380430375	9038907574	9309859154	90000075219	0.00012
35	9443014514	1870711823	5436619718	30000075219	0.00010
36	9004310792	4135202663	0471830985	91500000752	19400256282756e-05
37	9521692414	4331407110	4591549295	77400000752	19322351782782e-05
38	6279094142	2683534286	3957605633	80200000752	19784314464717e-05
39	9187958471	3804260106	1281690140	84000000752	19168930605272e-05
40	3089980002	3509691547	3467605633	80200000752	19751406263163e-05
41	0424898978	2004747135	5371830985	91500000752	19801862449629e-05
42	3137737935	5730248491	5209154929	57700000752	19329989034106e-05
43	9669521547	1394594864	1043661971	83000000752	19323688349516e-05
44	7420962856	6166855650	8871830985	91500000752	19878527937163e-05
45	4592332686	1350518548	9947887323	94300000752	19870926211617e-05
46	0876736794	7218939646	86 62.50000	00000075219	209717842259e-06
47	4156713024	2020514259	8757605633	80200000752	19873178278196e-06
48	1578273773	1016880089	1257605633	80200000752	19246713805587e-06
49	8574436249	2070670826	3357605633	80200000752	19178929321103e-07

4. Slurm file explanations

- We merge the following two key parts in one Slurm file
  - Slurm script
  - Singularity command
- Some people put the Singularity command as an external shell script called by sbatch script.

4.1 Slurm script explanations

- Slurm (the workload manager) provides sbatch, srun, and salloc for submitting and running jobs on a cluster.
- **sbatch**: It submits a batch job script to Slurm's scheduler.
- **srun**: srun launches tasks (parallel steps) within a job or allocation. The terminal should be always online; or the training will be stopped.

4.1 Slurm directives

- We explain key parts in this section.
- --partition: dev, normal, and normal2
- dev has less resources, but could be scheduled quickly.
- Please read the table below.
- Change to normal later.

```
#!/bin/bash
#SBATCH --job-name=cls-sing
#SBATCH --partition=dev
#SBATCH --account=MSTXXXX     ## iService_ID
## 選一種 GPU 申請方式（依叢集設定）
# 新版寫法（若支援）
##SBATCH --gpus=1
# 通用寫法（多數中心可用）
#SBATCH --gres=gpu:1
#SBATCH --cpus-per-task=8
#SBATCH --time=01:00:00
```

佇列	每個計劃最多可用 GPU 總數	每個 Job 最大執行時間	同時執行 job 數上限	佇列等候（排隊）數上限	GPU 型號
dev	8	2 小時	2	2	H100
normal	16	48 小時	2	2	H100
normal2	16	48 小時	2	2	H200

4.1 Slurm directives

- --gpus: Number of GPU 1 to 8
- -- gres: Number of GPU 1 to 8
- --cpus-per-task: CPU cores
- --time could be changed later.

```
#!/bin/bash
#SBATCH --job-name=cls-sing
#SBATCH --partition=dev
#SBATCH --account=MSTXXXX     ## iService_ID
## 選一種 GPU 申請方式（依叢集設定）
# 新版寫法（若支援）
##SBATCH --gpus=1
# 通用寫法（多數中心可用）
#SBATCH --gres=gpu:1
#SBATCH --cpus-per-task=8
#SBATCH --time=01:00:00
#SBATCH --output=%x-%j.out
#SBATCH --error=%x-%j.err
```

4.2 User-tunable variables

- **CONTAINER**="/work/hpc_sys/sifs/pytorch_23.11-py3.sif" – Path to the Singularity container image used for the job. The details are shown in **Section 4.2.1** to **4.2.3**.
- DATA_DIR="${HOME}/NCHC-Slurm-Demo/data/diabetic-retinopathy" – Directory containing training/validation/test data.
- SRC_DIR="${HOME}/" – Base source directory where your code/repos live.
- TIMM_DIR="${SRC_DIR}/NCHC-Slurm-Demo/pytorch-image-models" – Path to the local timm (pytorch-image-models) source tree.
- EPOCHS=50 – Number of training epochs.
- IMG_H=512, IMG_W=512 – Input image height and width fed to the model.
- BATCH=64 – Training batch size.
- WORKERS=${SLURM_CPUS_PER_TASK:-4} – Number of DataLoader worker processes (defaults to cpus-per-task).

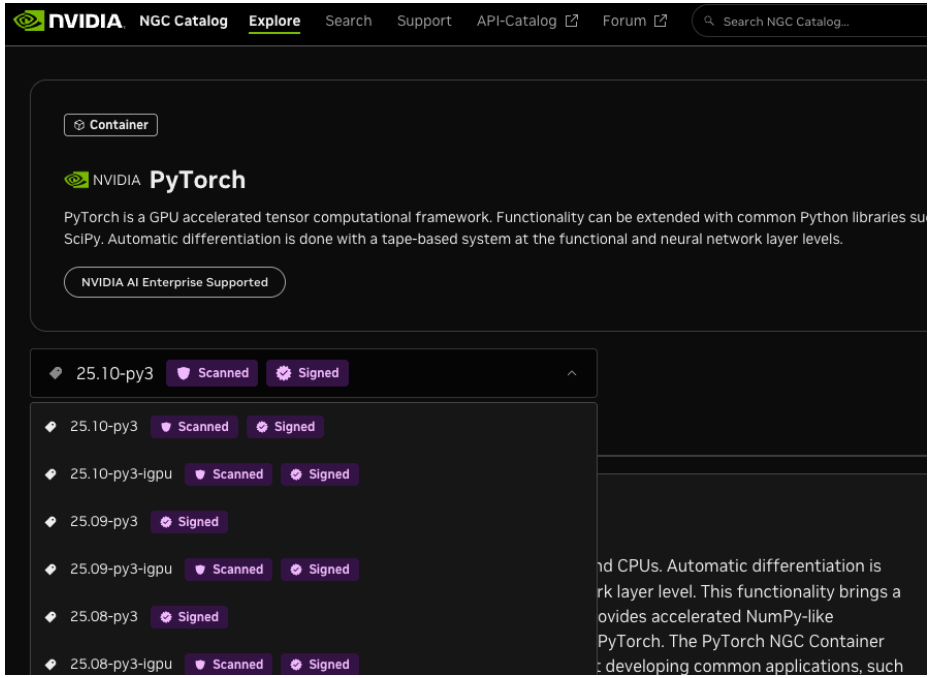
4.2.1 Singularity Container Image

- CONTAINER environment is available from "/work/hpc_sys/sifs/pytorch_23.11-py3.sif”
- How to select other SIF files?
- **Method 1**: Obtain other older SIFs under "/work/hpc_sys/sifs/” .
  - pytorch_22.05-py3.sif
  - pytorch_22.09-py3.sif
  - pytorch_22.09-py3_horovod.sif
  - pytorch_22.11-py3.sif
  - pytorch_23.02-py3_horovod.sif

4.2.1 Singularity Container Image

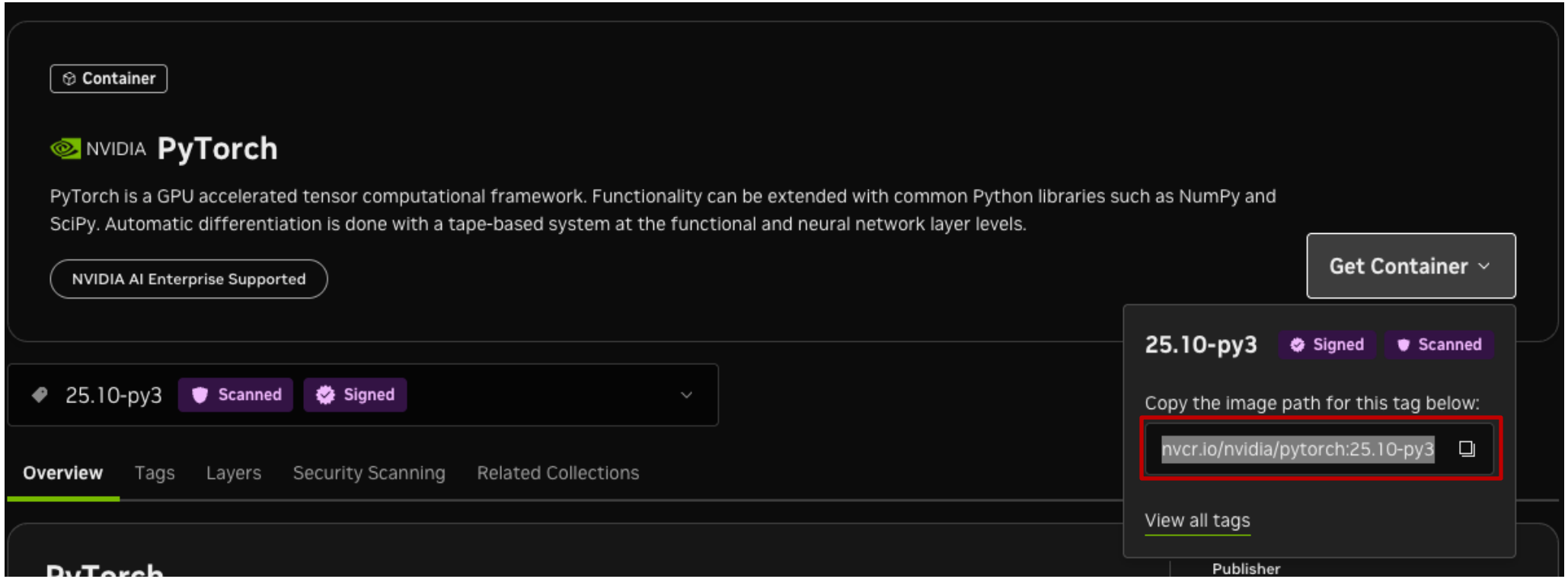
- **Method 2: Apply the nVidia NGC**
- Step 1: Find the exact tag you want
- PyTorch and Tensorflow images packed by nVidia

https://catalog.ngc.nvidia.com/orgs/nvidia/containers/pytorch
https://catalog.ngc.nvidia.com/orgs/nvidia/containers/tensorflow



4.2.1 Singularity Container Image

- Step 2: Copy the image path



4.2.1 Singularity Container Image

- Step 3: Pull the image by singularity (Called apptainer since 2021) on Nano5
- # General pattern
- singularity pull pytorch_<TAG>.sif docker://nvcr.io/nvidia/pytorch:<TAG>

- # Examples
- singularity pull pytorch_25.10-py3.sif docker://nvcr.io/nvidia/pytorch:25.10-py3

4.2.2 Build your own Container Image

- NGC container sometimes doesn’t install the package we need, such as the libGL is used in YOLO.
- If you build the image including the required package, it should save time and budget.
- How to build the image is out of the scope of this slides.

4.3 Env / runtime settings

- module load singularity – Loads Singularity/Apptainer module so container commands work.
- export OMP_NUM_THREADS=${WORKERS} – Sets OpenMP thread count (used by many math libs).
- export MKL_NUM_THREADS=${WORKERS} – Sets number of threads for Intel MKL operations.
- export PATH="${HOME}/.local/bin:${PATH}" – Ensures user-installed Python tools in ~/.local/bin are found.

4.4 srun + container execution

- srun singularity exec --nv – Run the job under Slurm inside the container with GPU access enabled.
- -B "${HOME}:${HOME}" – Bind-mounts your home directory into the container.
- --env DATA_DIR=...,EPOCHS=...,IMG_H=...,IMG_W=...,BATCH=...,WORKERS=... – Passes training hyperparameters into the container environment.

4.5 Adapt to another task

- You might like to train the object detection or LLM
- User variables section: Change the source code, dataset path, hyper parameters (epoch, batch size, and so on).
- Code setup inside the container: Replace the “install timm + basic libs” part with the dependent libraries.
- Training command: Swap the train.py (timm) invocation to your training script, passing specific options (e.g., model config, data yaml, image size).

5. Conclusions

- A good starting point to run algorithms on NCHC, particularly the deep learning on the Nano5.
- Nano5 could provide a great value for the deep learning research
- We could reduce the fee to buy the GPU which is not always run 365 days.
- This platform enhances the speed, flexibility, and our imaginations.

5.1 What is the next?

- Run your algorithms and dataset
- Enable the automatic mixed precision (AMP) during the forward pass during training.
- Use the Mobile App OTP Push instead of the Email OTP