



## 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

- **Performance and Hourly Pricing on NCHC**

NCHC Platform	GPU Spec	FP32 TFLOPS	TF32 TFLOPS	FP16 TFLOPS	NSTC	Academic
Nano5	H100 80GB	67	989 <sup>*1</sup>	1979	\$25	\$50
Nano5	H200 141GB	67	989 <sup>*1</sup>	1979	\$30	\$60
Forerunner1	A40 48 GB	37.4	74.8	149.7	\$0.1 * CPUs <sup>*2</sup>	\$0.2 * CPUs
TWCC	V100 32GB	15.7	-	125	\$10	\$20
-	RTX 5090 32GB	104.8	104.8/209.5 <sup>*3</sup>	209.5/419	-	-

- H100 has a better cost-performance ratio than V100.
- Forerunner1 (創進一號) provides a little GPUs. But the price is quite competitive.

<sup>\*1</sup> TF32 is on automatically without revising the code (e.g., loss scaling). Manually control of the TF32 is shown in the right.

<sup>\*2</sup> Forerunner1 only charges the CPU cores while A40 is not charged!

<sup>\*3</sup> RTX 5090 Tensor Performance detail: <https://images.nvidia.com/aem-dam/Solutions/geforce/blackwell/nvidia-rtx-blackwell-gpu-architecture.pdf>

```
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.

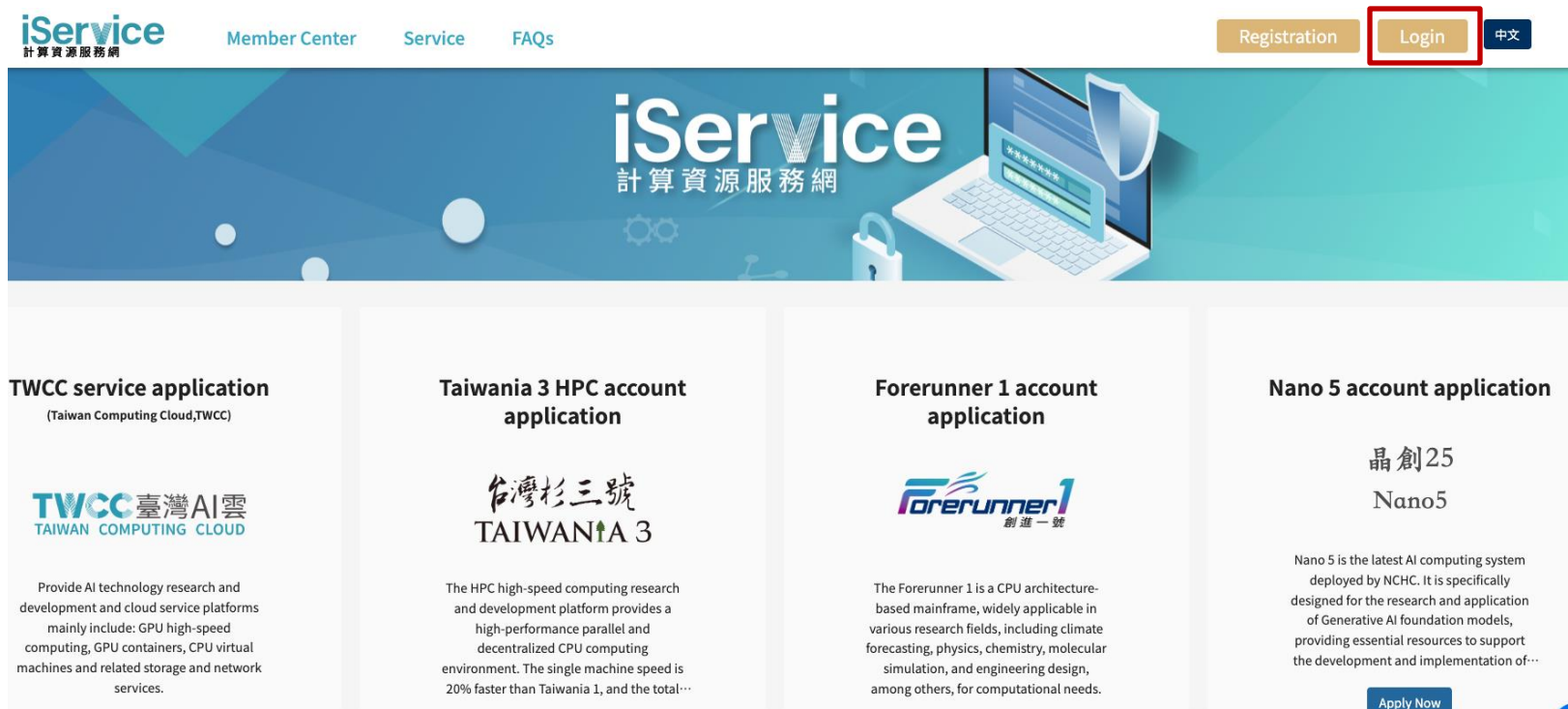
## 2. Login to Nano5 Server

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



## 2.1 Set the server password

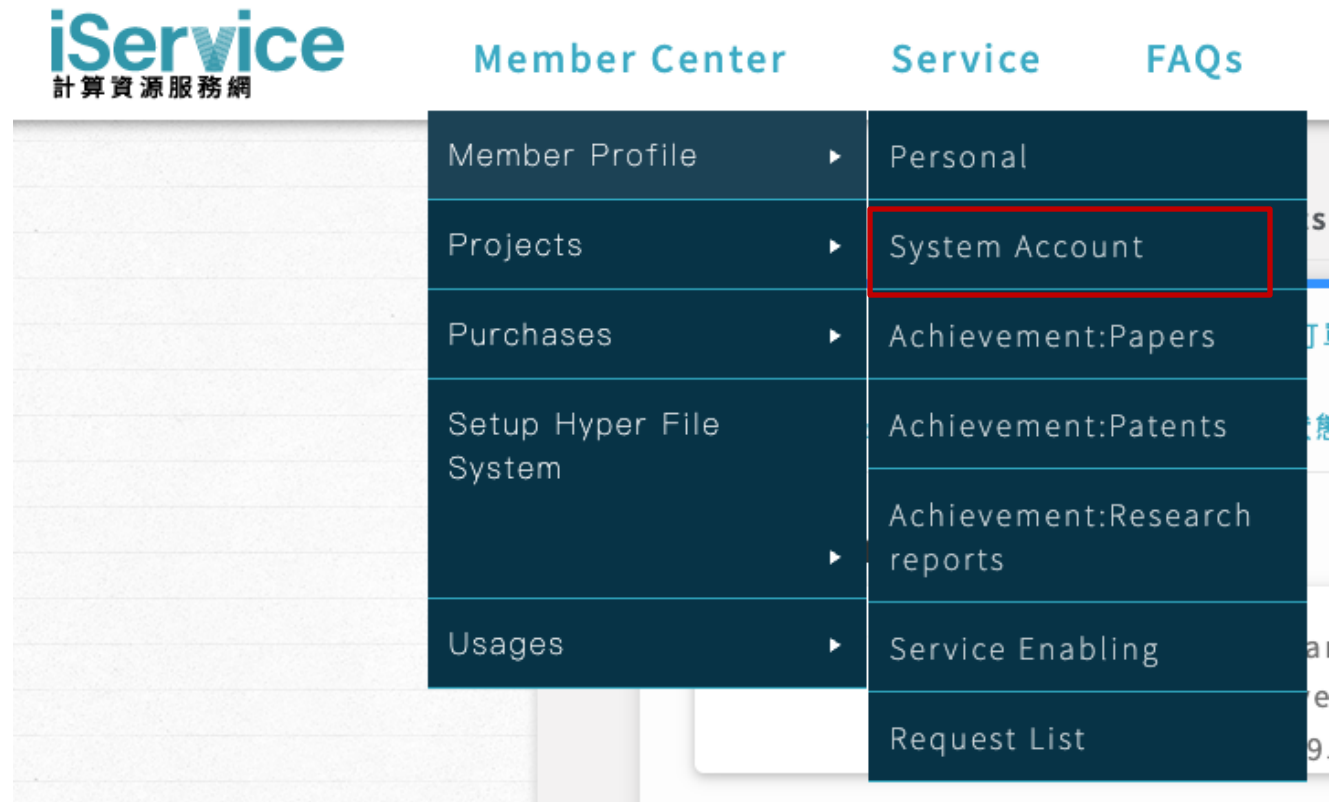
- Step 1: Login to HCHC Service Portal
- [https://iservice.nchc.org.tw/nchc\\_service/index.php](https://iservice.nchc.org.tw/nchc_service/index.php)





## 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” if you forgot the password.
- Step 6 : Turn on the OTP. OTP by mobile App for faster 2-factor authentication.

Member Center   Service   FAQs

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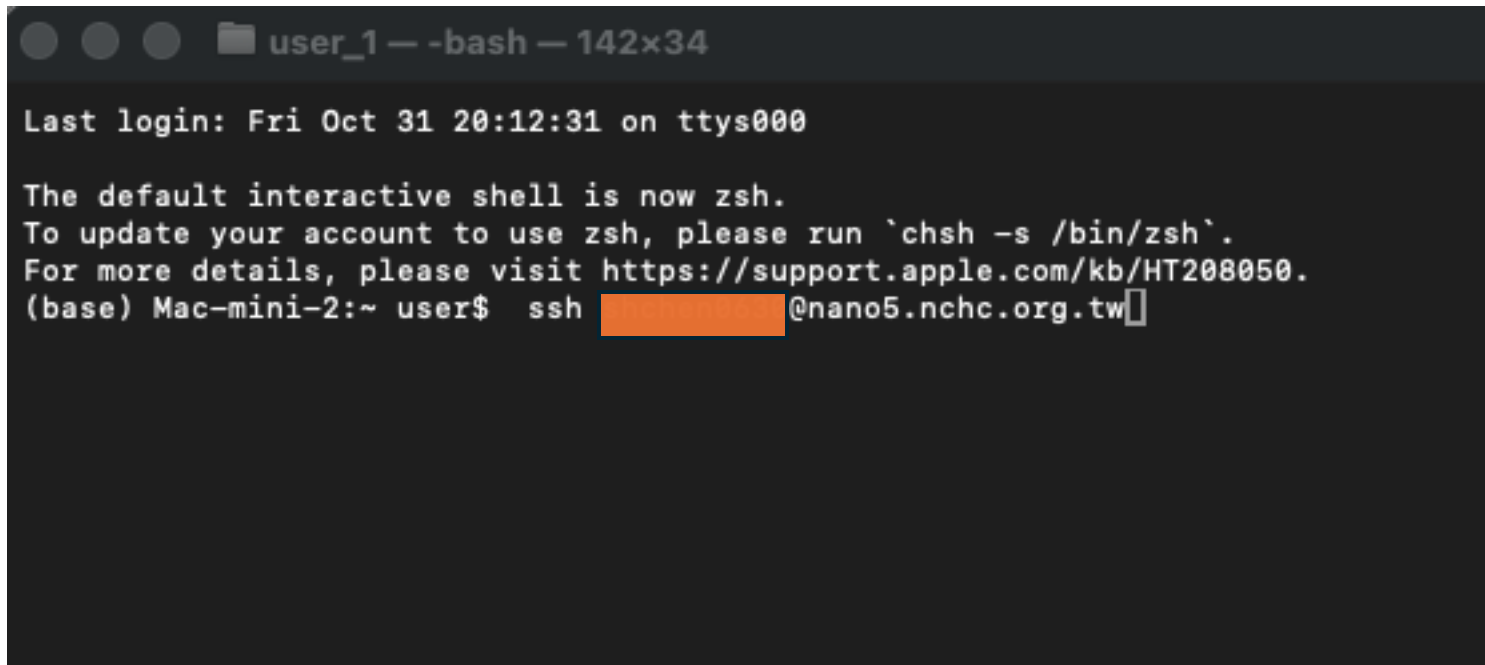
Modify the basic information of the supercomputer account.

**Supercomputer account**

Supercomputer account <div><div></div>(enable)</div>	Supercomputer password <div>change unix account password</div> <div> :::Date of last supercomputer password change. : 2025-10-31 20:19:53</div>	OTP Token: Valid <div>delete user otp</div> <div>Date of last successful MOTP token deletion : 無</div>
---	--	---

## 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.

A terminal window titled 'user\_1 — -bash — 142x34' showing the output of an SSH connection. The text displayed is: 'Last login: Fri Oct 31 20:12:31 on ttys000', 'The default interactive shell is now zsh.', 'To update your account to use zsh, please run `chsh -s /bin/zsh`.', 'For more details, please visit https://support.apple.com/kb/HT208050.', and '(base) Mac-mini-2:~ user\$ ssh [redacted]@nano5.nchc.org.tw'.

```
user_1 — -bash — 142x34
Last login: Fri Oct 31 20:12:31 on ttys000

The default interactive shell is now zsh.
To update your account to use zsh, please run `chsh -s /bin/zsh`.
For more details, please visit https://support.apple.com/kb/HT208050.
(base) Mac-mini-2:~ user$ ssh [redacted]@nano5.nchc.org.tw
```

## 2.2 Connection by SSH client

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

```
[(base) Mac-mini-2:~ user$ ssh shchen0630@nano5.nchc.org.tw
(shchen0630@nano5.nchc.org.tw) Please select the 2FA login method.
1. Mobile APP OTP
2. Mobile APP PUSH
3. Email OTP
Login method: 3
```

## 2.2 Connection by SSH client

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

[NCHC iService 服務網]登入驗證碼通知信，此密碼將於2025-11-02 1

◆ Summarize this email



國家高速網路與計算中心

to me ▾

您好：

412289 為您的[NCHC iService 服務網] 登入驗證碼，

您於 2025-11-02 19:07:10 使用主機帳號 [redacted] 登入 140.110.148.3，

此密碼將於 2025-11-02 19:10:10 內有效。

如果您未提交驗證請求，敬請儘速向本中心反應。

```
[(base) Mac-mini-2:~ user$ ssh [redacted]@nano5.nchc.org.tw
([redacted]@nano5.nchc.org.tw) Please select the 2FA login method.
1. Mobile APP OTP
2. Mobile APP PUSH
3. Email OTP
Login method: 3
([redacted]@nano5.nchc.org.tw) Password:
([redacted]@nano5.nchc.org.tw) OTP: 412289
```



## 2.2 Connection by SSH client

- Step 4: Login successfully!

[illegible]

## 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.



輸入密碼

請輸入此伺服器的密碼:

名稱: TWCC-Nano5

主機: nano5.nchc.org.tw:2222

使用者:

需要確認:

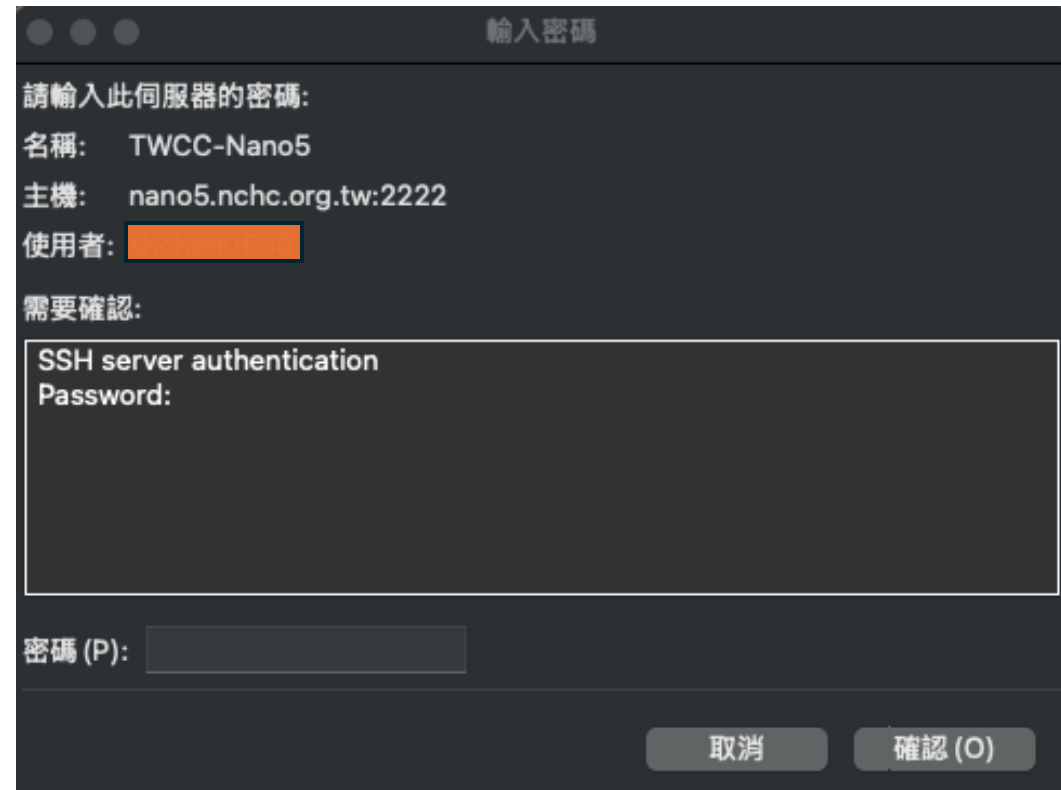
SSH server authentication

Please select the 2FA login method. 1. Mobile APP OTP 2. Mobile APP PUSH

3. Email OTP Login method:

密碼 (P):

取消 確認 (O)



輸入密碼

請輸入此伺服器的密碼:

名稱: TWCC-Nano5

主機: nano5.nchc.org.tw:2222

使用者:

需要確認:

SSH server authentication

Password:

密碼 (P):

取消 確認 (O)

## 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>

📁 Versions

Use this Dataset ▾ Use this Model ▾

**Versions**

2023-04-19 12:45am ✓

v1 2838

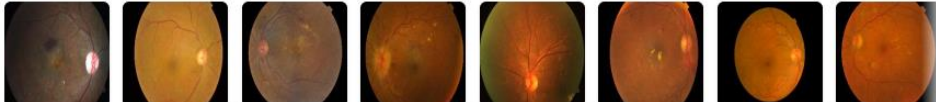
**v1 2023-04-19 12:45am**

Generated on Apr 19, 2023

[Download Dataset](#)

2838 Total Images

[View All Images →](#)



**Dataset Split**

TRAIN SET	70%	VALID SET	20%	TEST SET	10%
1986 Images		568 Images		284 Images	

**Preprocessing**

Auto-Orient: Applied  
Resize: Fit within 192x192

## 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: Congratulations! You obtain a job ID as the response.



## 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.
  - `queue -u YOUR_ACCOUNT`
- Step 6: Read the output log: `cls-sing-XXXXX.out`

```
+-----+
| NVIDIA-SMI 550.127.08                Driver Version: 550.127.08      CUDA Version: 12.4      |
+-----+-----+-----+-----+-----+-----+
| GPU  Name      Persistence-M | Bus-Id  Disp.A | Volatile Uncorr. ECC |
| Fan  Temp      Perf          |            Memory-Usage | GPU-Util  Compute M. |
|               Pwr:Usage/Cap |      1MiB / 81559MiB |           MIG M.     |
+-----+-----+-----+-----+-----+-----+
|  0   NVIDIA H100 80GB HBM3   | 00000000:BC:00:0 Off |           0         |
| N/A   28C      P0              | 1MiB / 81559MiB | 0%          Default |
+-----+-----+-----+-----+-----+-----+

+-----+
| Processes: |
| GPU   GI    CI      PID    Type    Process name                        GPU Memory |
|   ID   ID     ID              |                 | Usage    |
+-----+-----+-----+-----+-----+-----+
| No running processes found |
+-----+

pip 25.3 from /home, .local/lib/python3.10/site-packages/pip (python 3.10)
Looking in indexes: .org/simple, https://pypi.ngc.nvidia.com
Requirement already satisfied: pip==25.3 in /home/shchen0630/.local/lib/python3.10/site-packages (25.3)
pip 25.3 from /home, .local/lib/python3.10/site-packages/pip (python 3.10)
Looking in indexes: .org/simple, https://pypi.ngc.nvidia.com
Requirement already satisfied: pip in /home/shchen0630/.local/lib/python3.10/site-packages (25.3)
Looking in indexes: https://pypi.org/simple, https://pypi.ngc.nvidia.com
Requirement already satisfied: wheel in /home/shchen0630/.local/lib/python3.10/site-packages (0.45.1)
Requirement already satisfied: setuptools in /home/shchen0630/.local/lib/python3.10/site-packages (80.9.0)
Looking in indexes: https://pypi.org/simple, https://pypi.ngc.nvidia.com
Requirement already satisfied: pip in /home/shchen0630/.local/lib/python3.10/site-packages (25.3)
```

## 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, maxin
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: 1.000e-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	93275759297976230675021830985915	00000075219	0.00019			
30	565259579680015528638573943661971	00000075219	0.00017			
31	61474738582996697412409154929577	00000075219	0.00016			
32	10147726151349715300009154929577	00000075219	0.00014			
33	06468450638322312046167605633802	00000075219	0.00013			
34	103804303759038907574933098591549	00000075219	0.00012			
35	944301451401870711823543661971830	00000075219	0.00010			
36	900431079241352026630471830985915	00000075219	400256282756e-05			
37	952169241443314071104591549295774	00000075219	22351782782e-05			
38	62790941422683534286357605633802	00000075219	784314464717e-05			
39	91879584713804260106128169014084	00000075219	168930605272e-05			
40	308998000235096915473467605633802	00000075219	751406263163e-05			
41	042489897820047471355371830985915	00000075219	801862449629e-05			
42	31377379355730248491529154929577	00000075219	329989034106e-05			
43	966952154713945948641043661971830	00000075219	323688349516e-05			
44	742096285661668556508871830985915	00000075219	878527937163e-05			
45	459233268613505185489547887323943	00000075219	870926211617e-05			
46	087673679472189396468662.50000	00000075219	209717842259e-06			
47	41567130242205142598757605633802	00000075219	873178278196e-06			
48	15782737730168800891257605633802	00000075219	246713805587e-06			
49	85744362492070670826357605633802	00000075219	78929321103e-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=MSTXXX    ## 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 **4.2.2**.
- **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:-8} – Number of DataLoader worker processes (defaults to cpus-per-task).

## 4.2.1 Existing Singularity Container Images

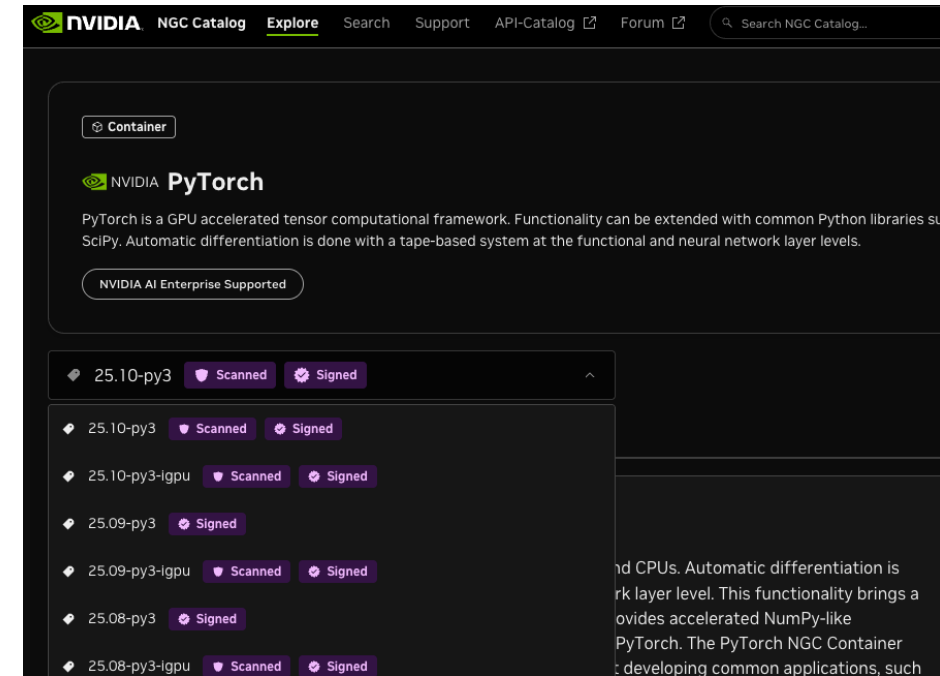
- CONTAINER environment is available from `"/work/hpc_sys/sifs/pytorch_23.11-py3.sif"`
- How to select other SIF files?
- **Method 1:** Obtain other older SIFs under `"/work/hpc_sys/sifs/"`.
  - `pytorch_22.05-py3.sif`
  - `pytorch_22.09-py3.sif`
  - `pytorch_22.09-py3_horovod.sif`
  - `pytorch_22.11-py3.sif`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

## 4.2.2 NGC 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>



## 4.2.2 NGC Singularity Container Image

- Step 2: Copy the image path

The screenshot shows the NVIDIA NGC container image page for PyTorch. The main header includes the NVIDIA logo, the text "PyTorch", and a description: "PyTorch is a GPU accelerated tensor computational framework. Functionality can be extended with common Python libraries such as NumPy and SciPy. Automatic differentiation is done with a tape-based system at the functional and neural network layer levels." Below this is a "Container" badge and a "Get Container" button. A dropdown menu shows the selected tag "25.10-py3" with "Scanned" and "Signed" status indicators. The "Overview" tab is active in the navigation bar. A modal window is open, displaying the tag "25.10-py3" and the instruction "Copy the image path for this tag below:". The image path "nvcr.io/nvidia/pytorch:25.10-py3" is highlighted in a red box, with a copy icon to its right. Below the path is a link to "View all tags".

Container

**NVIDIA PyTorch**

PyTorch is a GPU accelerated tensor computational framework. Functionality can be extended with common Python libraries such as NumPy and SciPy. Automatic differentiation is done with a tape-based system at the functional and neural network layer levels.

NVIDIA AI Enterprise Supported

Get Container ▾

25.10-py3 Signed Scanned

Copy the image path for this tag below:

`nvcr.io/nvidia/pytorch:25.10-py3`

[View all tags](#)

Overview Tags Layers Security Scanning Related Collections

PyTorch

Publisher

## 4.2.2 NGC 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.



## 4.3 Env / runtime settings

- CONTAINER\_CMD is the core of this script.
- It includes the package installations and the execution of the train.py
- The places should be revised for your own algorithm are shown in yellow.

**Note:** this command could be wrapped in a shell file and executed by srun. An example is shown below.  
[https://github.com/waue0920/nchc\\_hpc\\_slurm\\_example/tree/main/h100/example2\\_yolov9](https://github.com/waue0920/nchc_hpc_slurm_example/tree/main/h100/example2_yolov9)

```
CONTAINER_CMD=$(cat <<'EOS'  
set -euo pipefail
```

```
# 顯示 GPU 狀態 (確認 --nv 生效)  
nvidia-smi || true
```

```
# 準備程式碼目錄  
mkdir -p "$HOME/src"  
if [ ! -d "$HOME/src/pytorch-image-models" ]; then  
    git clone https://github.com/huggingface/pytorch-image-models.git  
    "$HOME/src/pytorch-image-models"  
fi
```

```
# upgrade pip to 25.3 (as requested), then deps  
python -m pip --version || true  
python -m pip install --user --upgrade "pip==25.3"  
python -m pip --version
```

```
# 安裝/更新必要套件到使用者空間 (寫入 $HOME/.local)  
python -m pip install --user --upgrade pip  
python -m pip install --user --upgrade wheel setuptools  
# timm 建議用原始碼; 另外也裝到 site-packages, 避免相依缺失  
python -m pip install --user --upgrade timm
```

```
# 進入 timm 原始碼目錄 (含 train.py)  
cd "$HOME/src/pytorch-image-models"
```

```
# 開始訓練 (單卡)  
python -u train.py "$DATA_DIR" \  
    --model convnext_base \  
    --epochs "$EPOCHS" \  
    --batch-size "$BATCH" \  
    --workers "$WORKERS" \  
    --input-size 3 "$IMG_H" "$IMG_W" \  
    --pin-mem --channels-last --amp \  
    --opt adamw --lr 5e-4 \  
    --aa rand-m9-mstd0.5 --mixup 0.2 --cutmix 1.0 \  
    --sched cosine  
EOS  
)
```

## 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
- Build your own image:
  - NGC container sometimes doesn't install the package we need, such as the libGL is used in YOLO.
  - You could build your own SIFs.