A use case of humanware and cloud-based CI: Time-series data classification using ML

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Outlines

1. Introduction
2. Using CI
3. Our Science Challenge
4. Implementations
5. Results
6. Humanware Discussion
7. Conclusions
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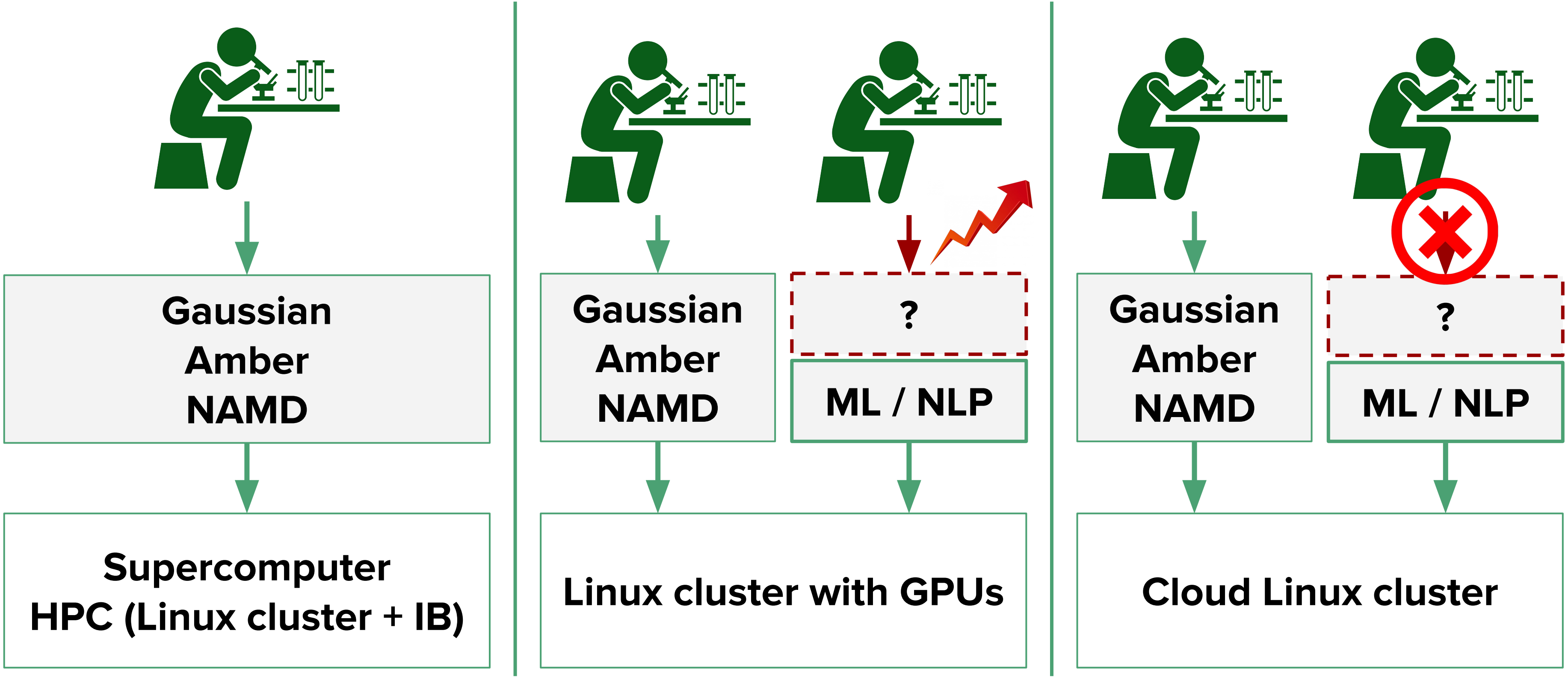
1.1 What is Cyberinfrastructure (CI) and Humanware?

Cyberinfrastructure (CI) can be defined as consisting of “… *computing systems, data storage systems, advanced instruments and data repositories, visualization environments,* ***and people****, all linked together by software and high-performance netw* *ductivity and enable breakthroughs not other*

Humanware[2]

- ➔ **Administering** physical component of CI
- ➔ **Support** researchers to utilize CI
- ➔ **Collaborate** with researchers
- ➔ Increase **efficiency**
- ➔ **Maximize** Return-On-Investment (ROI) of CI [6]
- ➔ Make **breakthrough** / Find **innovative** solutions

2.1 CI for researchers


Gaussian
Amber
NAMD

Supercomputer
HPC (Linux cluster + IB)

Gaussian
Amber
NAMD

?

ML / NLP

Linux cluster with GPUs

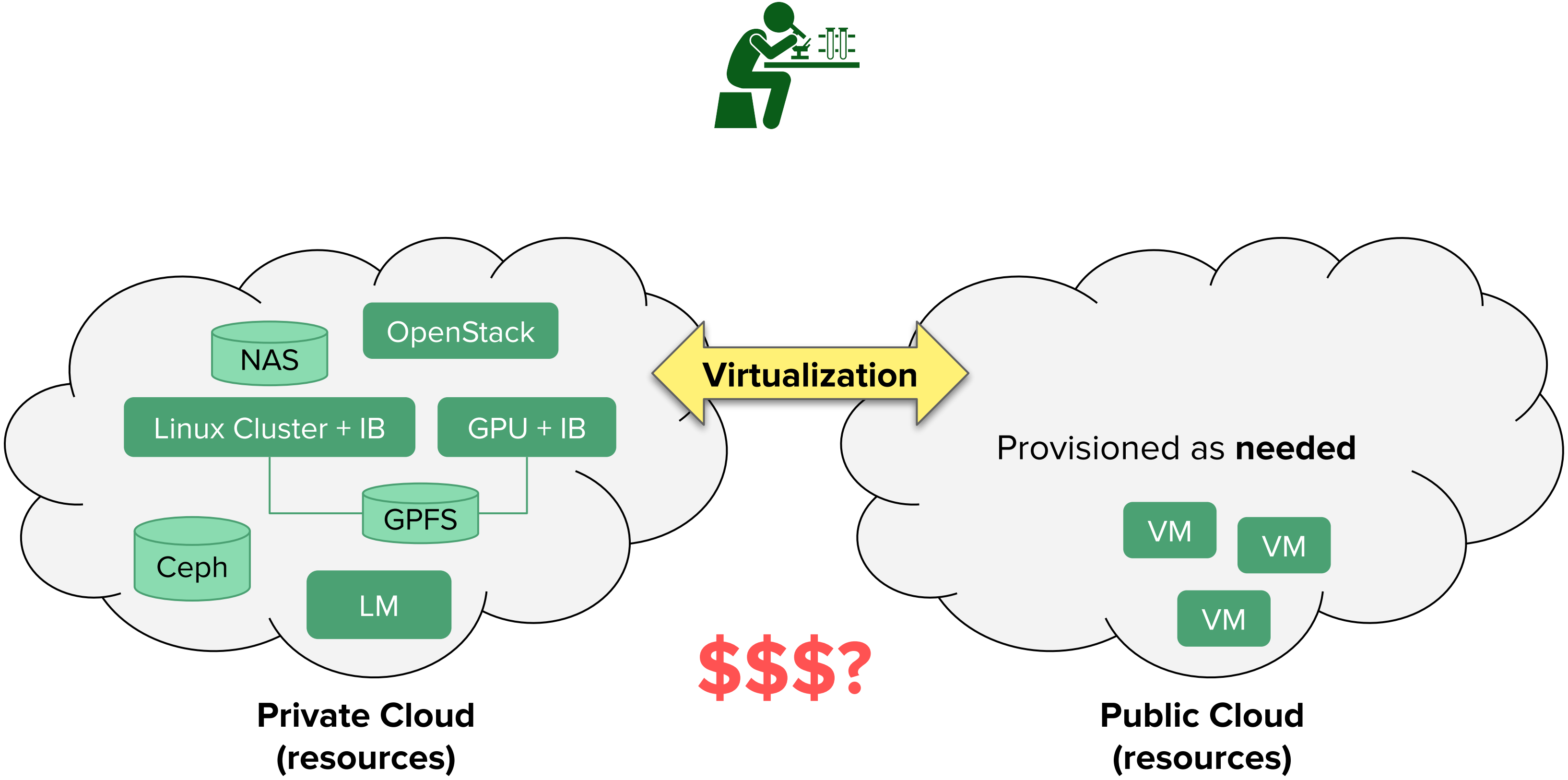
Gaussian
Amber
NAMD

?

ML / NLP

Cloud Linux cluster

2.2 Clouds complicate things


NAS
OpenStack
Linux Cluster + IB
GPU + IB
GPFS
Ceph
LM
Virtualization
Provisioned as **needed**
VM
VM
VM
$$$?
Private Cloud (resources)
Public Cloud (resources)

2.3 Cloud provisioning challenges

➔ Virtual Machine for Cloud-based CI

- ◆ **Operating System:** Windows? Linux? Distribution? Version?
- ◆ **CPU:** Number of CPUs?
- ◆ **GPU:** Number of GPUs? Nvidia-CUDA enabled?
- ◆ **RAM:** How large RAM?
- ◆ **Storage:** SSD? HDD? How large?
- ◆ **Network:** Requirement? How fast?

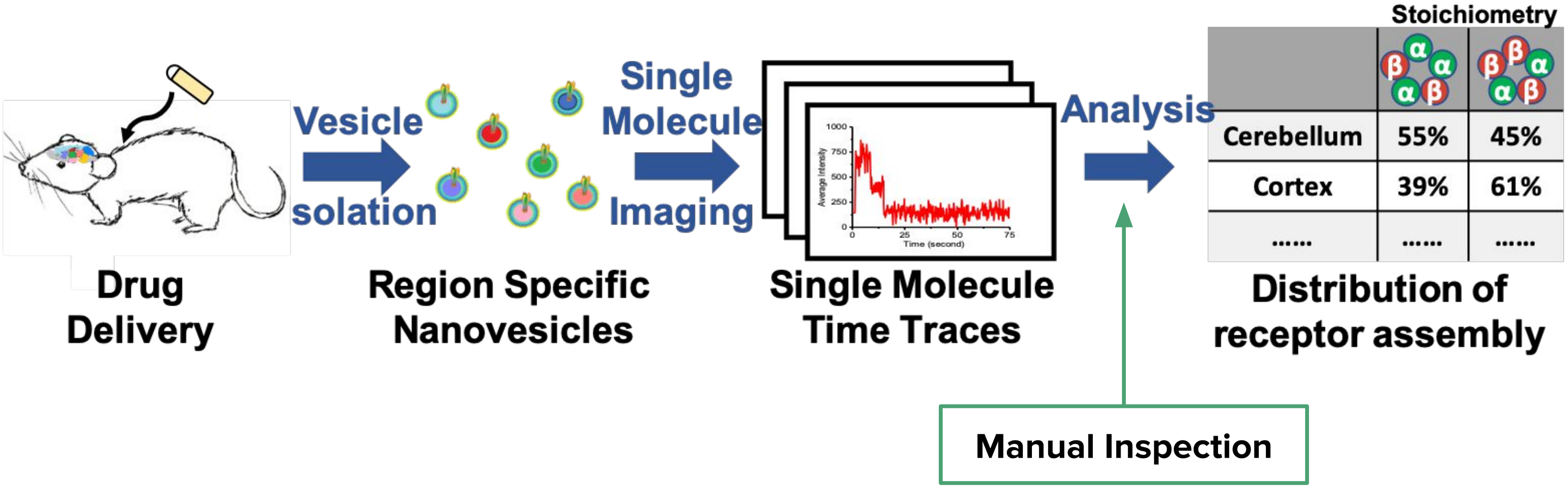
2.4 Cloud workflow challenges

- ➔ Move **data** in & out
  - ◆ scp / ssh / rclone
  - ◆ Git server
  - ◆ Dropbox / Google Drive
- ➔ **Sync** codes and data
  - ◆ Version control -- git / SVN / CVS
  - ◆ ~~**No version control!! -- Local disk / file servers / USB**~~
- ➔ Documentation
  - ◆ **Wiki** pages / How-to / Reports -- Google drive / Web pages / Project tracking tool
- ➔ Launching **pipeline** on data (stream processing)

2.5 Cloud programming challenges

- ➔ **Writing** machine learning codes
- ➔ What ML framework? (**Tensorflow / Keras / Pytorch / Theano**)
- ➔ Python, C++, R?
- ➔ Data **pre-processing**
- ➔ Data **post-processing**
- ➔ User interface?
- ➔ How to **manage** data, codes & results?
- ➔ How to **visualize** results?
- ➔ **Learning curve** for researchers

3.1 Our Science Challenge: Drug delivery (Chem/Pharm)



	Stoichiometry	
	α β α α β	β β α α β
Cerebellum	55%	45%
Cortex	39%	61%
......	......	......

Drug Delivery

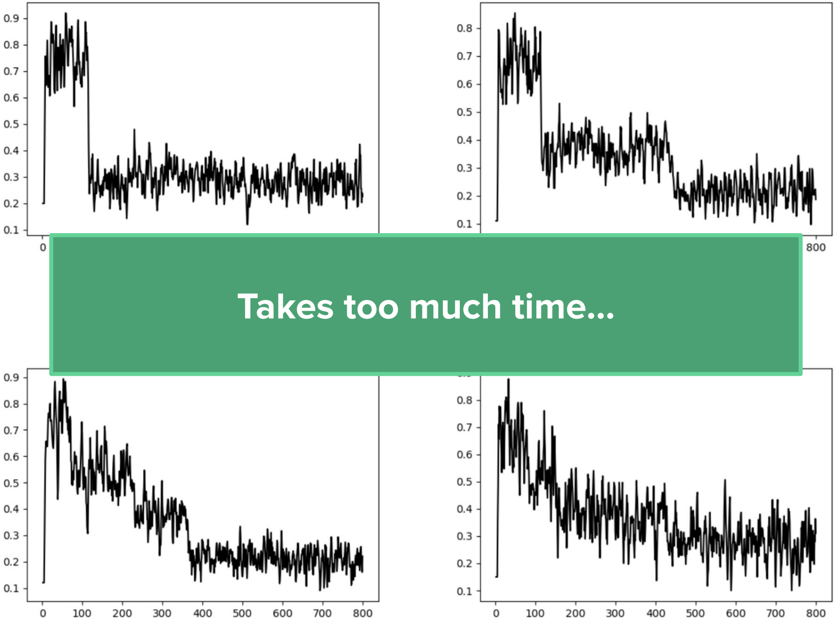
Region Specific Nanovesicles

Single Molecule Time Traces

Distribution of receptor assembly

Manual Inspection

3.2 Ambiguous Time-series Data



Takes too much time...

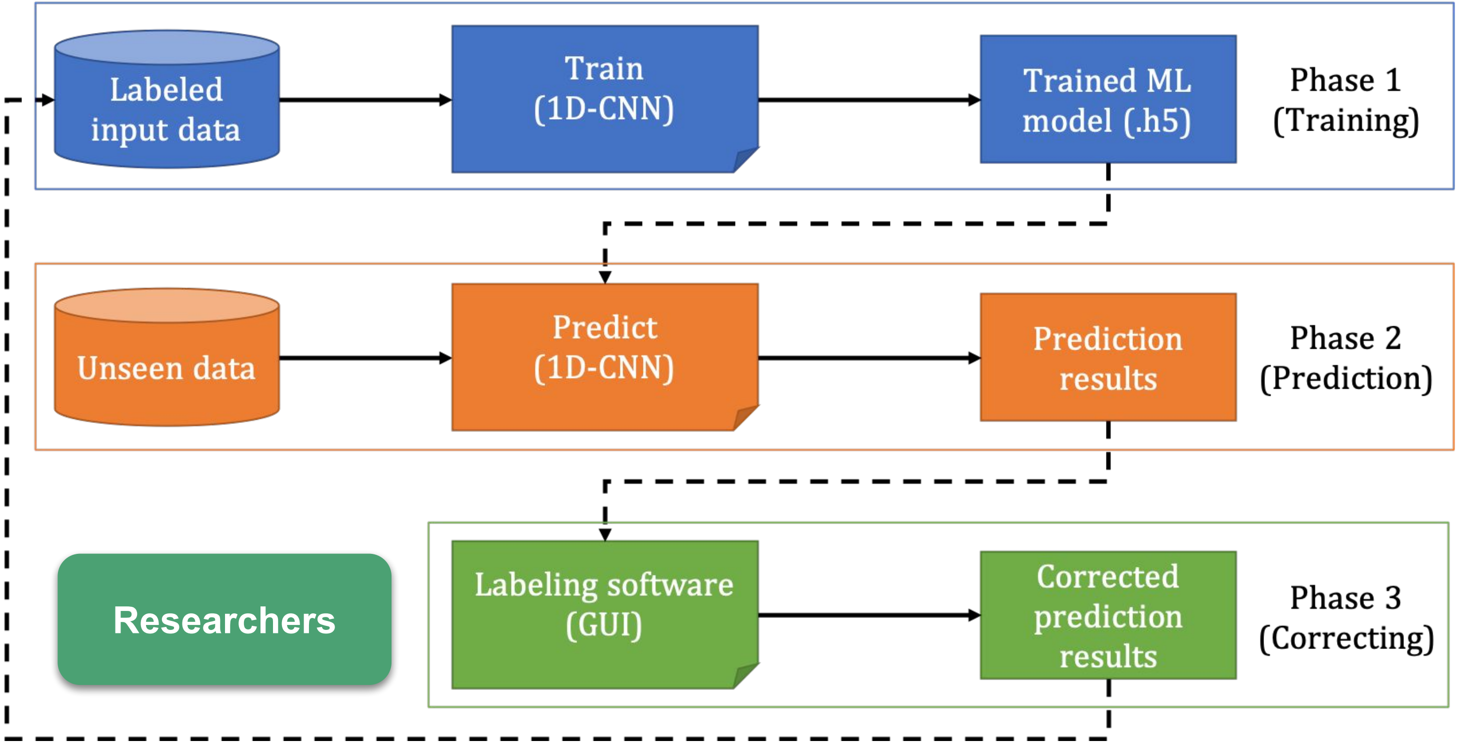
(c) 3 steps

(d) 0 steps

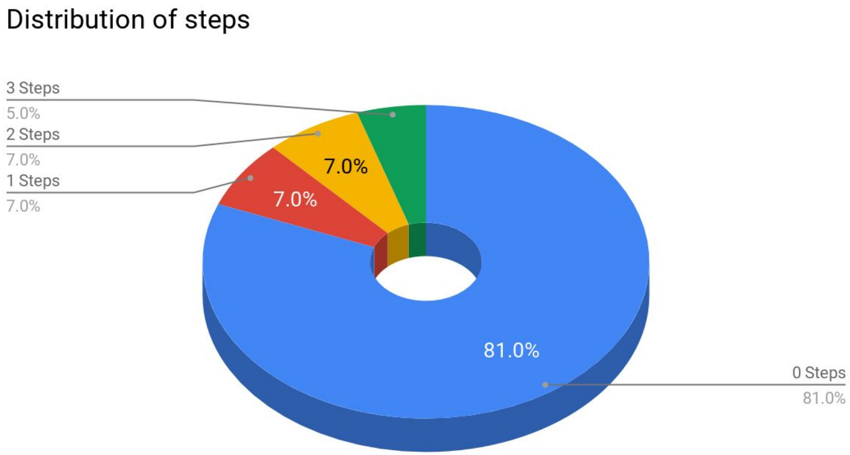
Figure 1: Example of actual data with correct labels

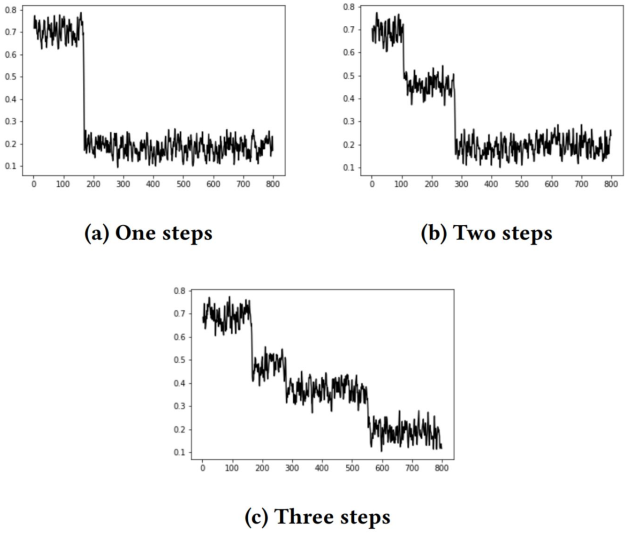
Machine Learning

4.1 Processing Pipeline



4.2 Augmentation for training phase





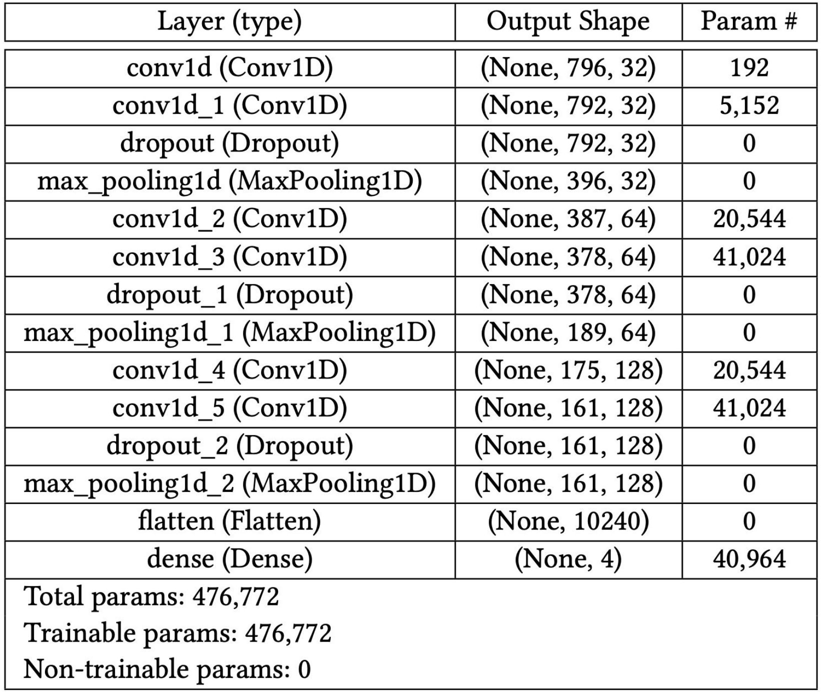
(a) One steps

(b) Two steps

(c) Three steps

Figure 4: Example of augmented data for 1, 2, and 3 steps

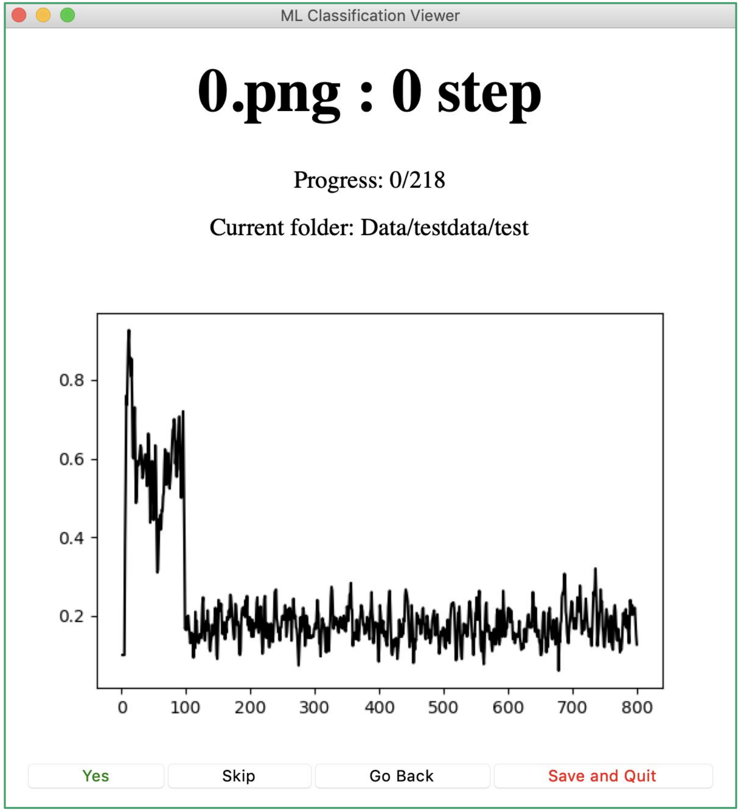
4.3 ML approaches / algorithm (1D-CNN)



Layer (type)	Output Shape	Param #
conv1d (Conv1D)	(None, 796, 32)	192
conv1d_1 (Conv1D)	(None, 792, 32)	5,152
dropout (Dropout)	(None, 792, 32)	0
max_pooling1d (MaxPooling1D)	(None, 396, 32)	0
conv1d_2 (Conv1D)	(None, 387, 64)	20,544
conv1d_3 (Conv1D)	(None, 378, 64)	41,024
dropout_1 (Dropout)	(None, 378, 64)	0
max_pooling1d_1 (MaxPooling1D)	(None, 189, 64)	0
conv1d_4 (Conv1D)	(None, 175, 128)	20,544
conv1d_5 (Conv1D)	(None, 161, 128)	41,024
dropout_2 (Dropout)	(None, 161, 128)	0
max_pooling1d_2 (MaxPooling1D)	(None, 161, 128)	0
flatten (Flatten)	(None, 10240)	0
dense (Dense)	(None, 4)	40,964

Total params: 476,772
Trainable params: 476,772
Non-trainable params: 0

4.4 Labeling GUI software



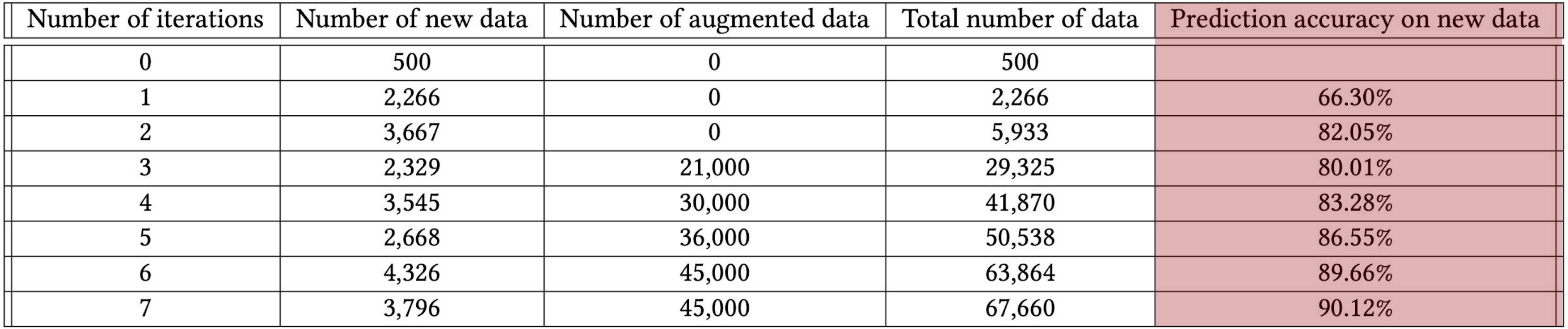
ML Classification Viewer

0.png : 0 step

Progress: 0/218

Current folder: Data/testdata/test

5.1 Records of training data and prediction accuracy

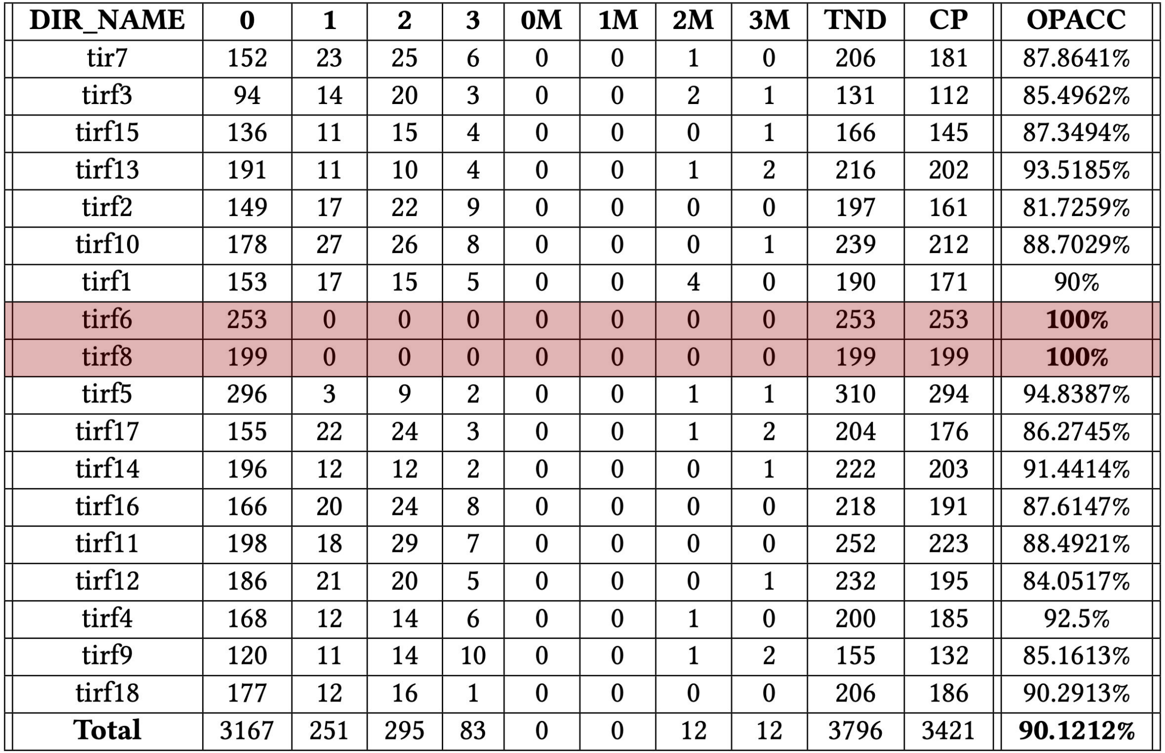


Number of iterations	Number of new data	Number of augmented data	Total number of data	Prediction accuracy on new data
0	500	0	500	
1	2,266	0	2,266	66.30%
2	3,667	0	5,933	82.05%
3	2,329	21,000	29,325	80.01%
4	3,545	30,000	41,870	83.28%
5	2,668	36,000	50,538	86.55%
6	4,326	45,000	63,864	89.66%
7	3,796	45,000	67,660	90.12%

Table 1: Records of training data size and prediction accuracy for iterations

- ➔ Each iteration takes a week (takes time to correct data by researchers)
- ➔ After 3rd iteration, we added augmented data set

5.2 Prediction results of the last iteration

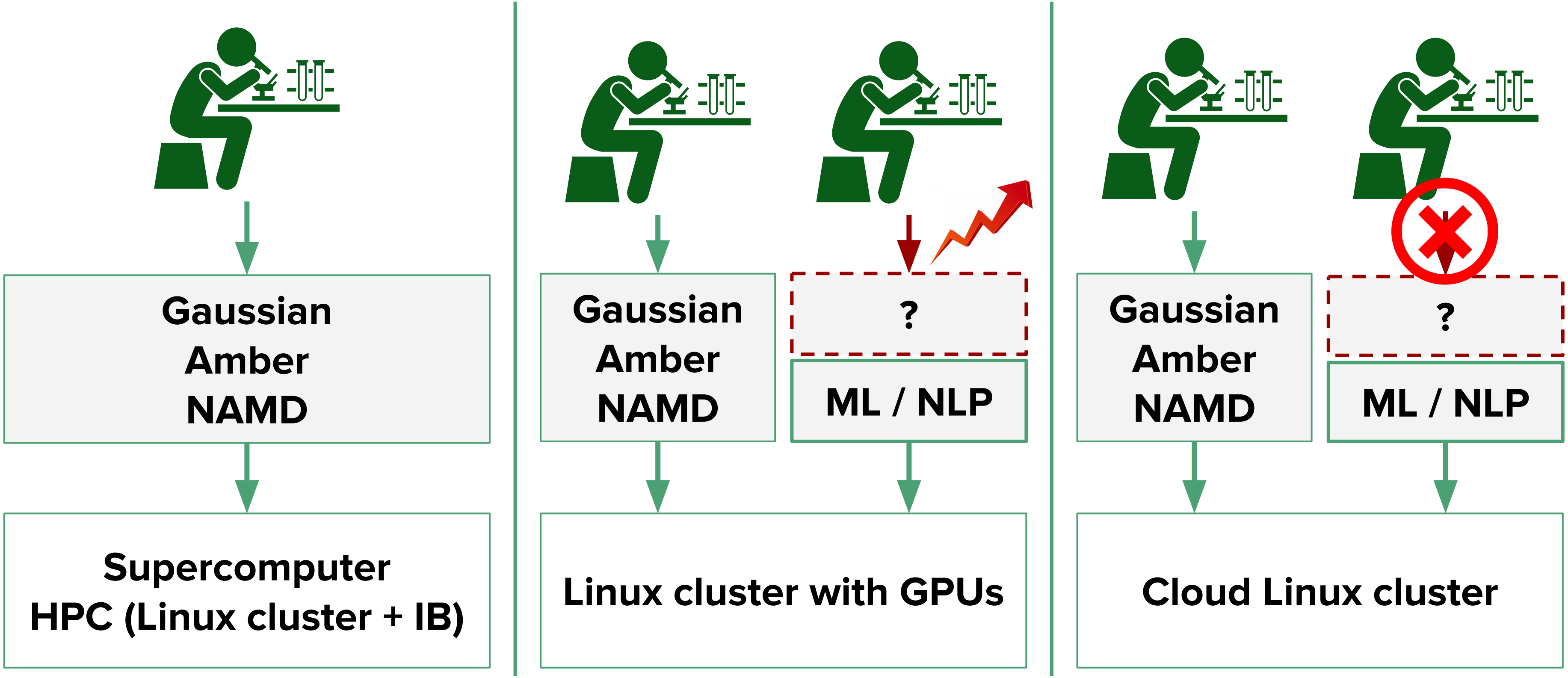


DIR_NAME	0	1	2	3	0M	1M	2M	3M	TND	CP	OPACC
tir7	152	23	25	6	0	0	1	0	206	181	87.8641%
tirf3	94	14	20	3	0	0	2	1	131	112	85.4962%
tirf15	136	11	15	4	0	0	0	1	166	145	87.3494%
tirf13	191	11	10	4	0	0	1	2	216	202	93.5185%
tirf2	149	17	22	9	0	0	0	0	197	161	81.7259%
tirf10	178	27	26	8	0	0	0	1	239	212	88.7029%
tirf1	153	17	15	5	0	0	4	0	190	171	90%
tirf6	253	0	0	0	0	0	0	0	253	253	**100%**
tirf8	199	0	0	0	0	0	0	0	199	199	**100%**
tirf5	296	3	9	2	0	0	1	1	310	294	94.8387%
tirf17	155	22	24	3	0	0	1	2	204	176	86.2745%
tirf14	196	12	12	2	0	0	0	1	222	203	91.4414%
tirf16	166	20	24	8	0	0	0	0	218	191	87.6147%
tirf11	198	18	29	7	0	0	0	0	252	223	88.4921%
tirf12	186	21	20	5	0	0	0	1	232	195	84.0517%
tirf4	168	12	14	6	0	0	1	0	200	185	92.5%
tirf9	120	11	14	10	0	0	1	2	155	132	85.1613%
tirf18	177	12	16	1	0	0	0	0	206	186	90.2913%
Total	3167	251	295	83	0	0	12	12	3796	3421	**90.1212%**

Table 3: Prediction results of the new data set in the seventh iteration

Humanware discussion

6.1 CI for researchers



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HPC (Linux cluster + IB)

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?

ML / NLP

Linux cluster with GPUs

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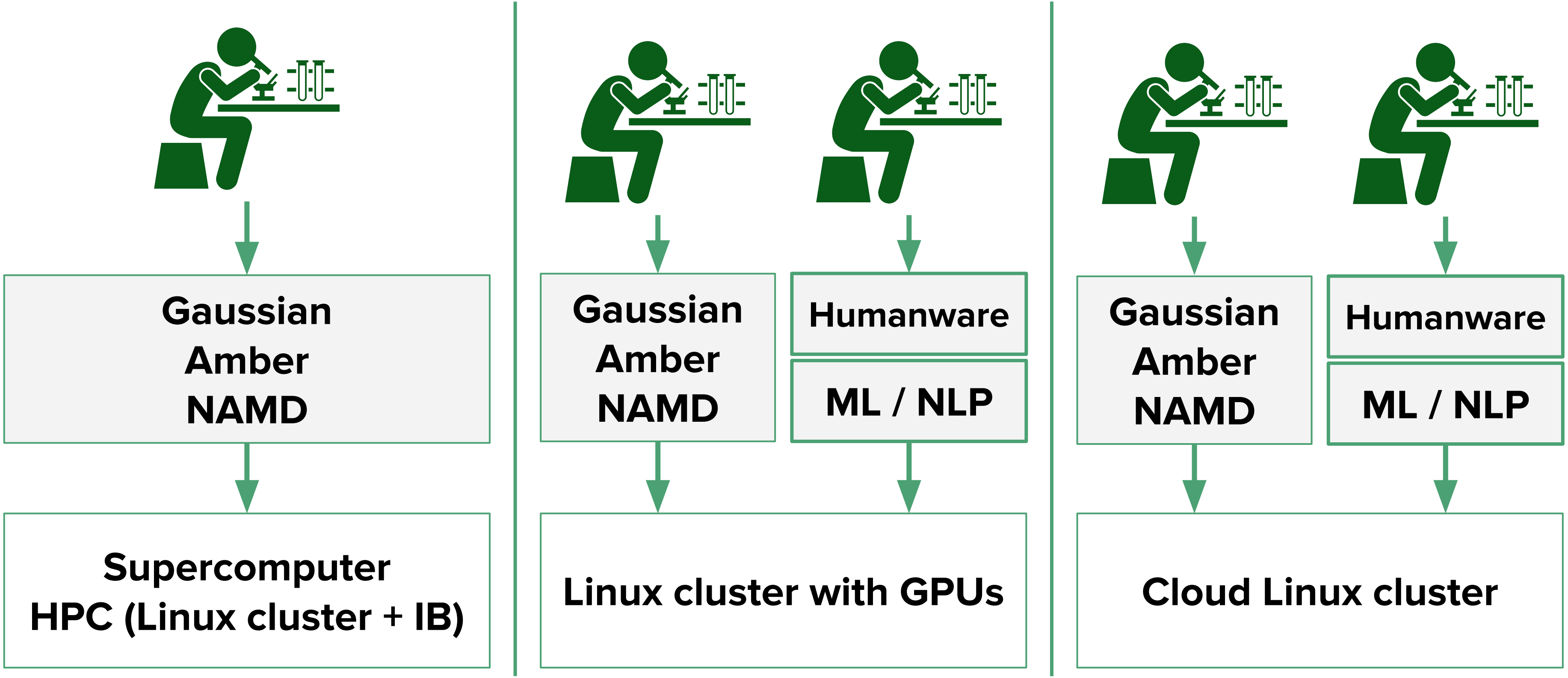
ML / NLP

Cloud Linux cluster

6.2 Humanware in the loop



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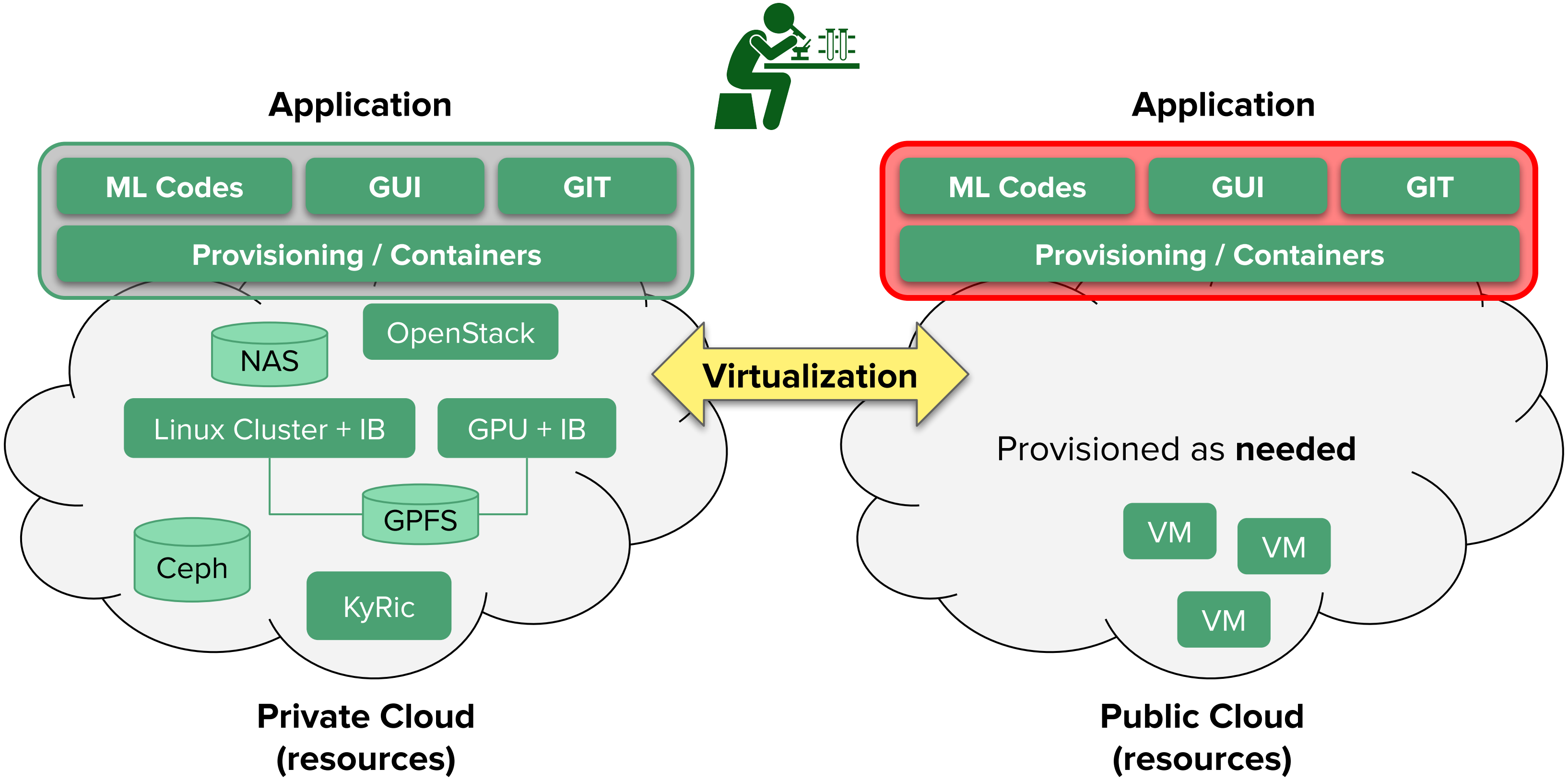
6.3 Moving to cloud CI



6.4 Cloud provisioning solutions

- Virtual Machine for Cloud-based CI
  - **Operating System:** Linux 16.04 LTS, 18.04 LTS
  - **CPU:** 6 x vCPUs
  - **GPU:** 1 x Nvidia Tesla M60 (8GB GPU memory)
  - **RAM:** 56GB
  - **Storage:** 340GB HDD + 512GB HDD
  - **Network:** Normal
  - **Cost**: NV6 Promo ($0.721 per hour + extra HDD = $200 per month)

6.5 Cloud workflow solutions

- Move **data** in & out
  - **Git server**
- **Sync** codes and data
  - **Version control -- git**
- Documentation
  - **Wiki** pages / How-to / Reports
  - Microsoft Azure Devops (https://ywsong2.visualstudio.com/Chem_ML_GUI)
- Launching **pipeline** on data (stream processing)
  - Training, Prediction, and Correction phases

6.6 Cloud programming solutions

- ➔ **Writing** machine learning codes (**1D-CNN**)
- ➔ What ML framework? (**Tensorflow / Keras / Nvidia CUDA**)
- ➔ Python? (**Anaconda** virtual environment)
- ➔ Data **pre- and post-processing** (Custom software)
- ➔ User interface? (Custom GUI software)
- ➔ How to **manage** data, codes & results? (Custom software)
- ➔ How to **visualize** results? (Custom software)

7.1 Conclusions

- ➔ **Clear need** for humanware as result of **new CI** and **research challenges**
- ➔ Many aspects of humanware component (**provisioning, workflow, programming, interfaces**)
- ➔ Possible to build **applications** that **hide details** for researchers
- ➔ Public cloud was **sufficient** and **usable** platform for our problem
- ➔ We could run in the **private cloud** with a few changes
- ➔ **Humanware** collaborates with researchers to **maximize** ROI of evolving CIs and make **breakthroughs**

QUESTIONS
ANSWERS

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