Progress on cloud native solution of Machine Learning as Service for HEP

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What is Machine Learning as a Service

Machine Learning as a Service (MLaaS) is used as an umbrella definition of various cloud-based platforms that provide a web service to users interested in ML tasks

- Leading **cloud providers** offer MLaaS solutions with different interfaces and APIs, designed to cover standard use cases, e.g. classification, regression, clustering, anomaly detection, performed in different sectors like natural language processing and computer vision.

- These **platforms** simplify and make ML accessible to even non-experts, ensuring affordability and scalability as these services inherit the strengths of the underlying cloud infrastructure. Moreover, the MLaaS solutions are well integrated with the rest of the provider's portfolio of services which thus offers a complete solution.

CLOUD MACHINE LEARNING SERVICES COMPARISON

	Amazon ML and SageMaker	Microsoft Azure AI Platform	Google AI Platform (Unified)	IBM Watson Machine Learning
Classification	✓	✓	✓	✓
Regression	✓	✓	✓	✓
Clustering	✓	✓	✓	✗
Anomaly detection	✓	✓	✗	✗
Recommendation	✓	✓	✓	✗
Ranking	✓	✓	✗	✗
Data Labeling	✓	✓	✓	✓
MLOps pipeline support	✓	✓	✓	✓
Built-in algorithms	✓	✓	✓	✗
Supported frameworks	TensorFlow, MXNet, Keras, Gluon. Pytorch, Caffe2, Chainer, Torch	TensorFlow, scikit-learn, PyTorch, Microsoft Cognitive Toolkit, Spark ML	TensorFlow, scikit-learn, XGBoost, Keras	TensorFlow, Keras, Spark MLlib, scikit-learn, XGBoost, PyTorch, IBM SPSS, PMML

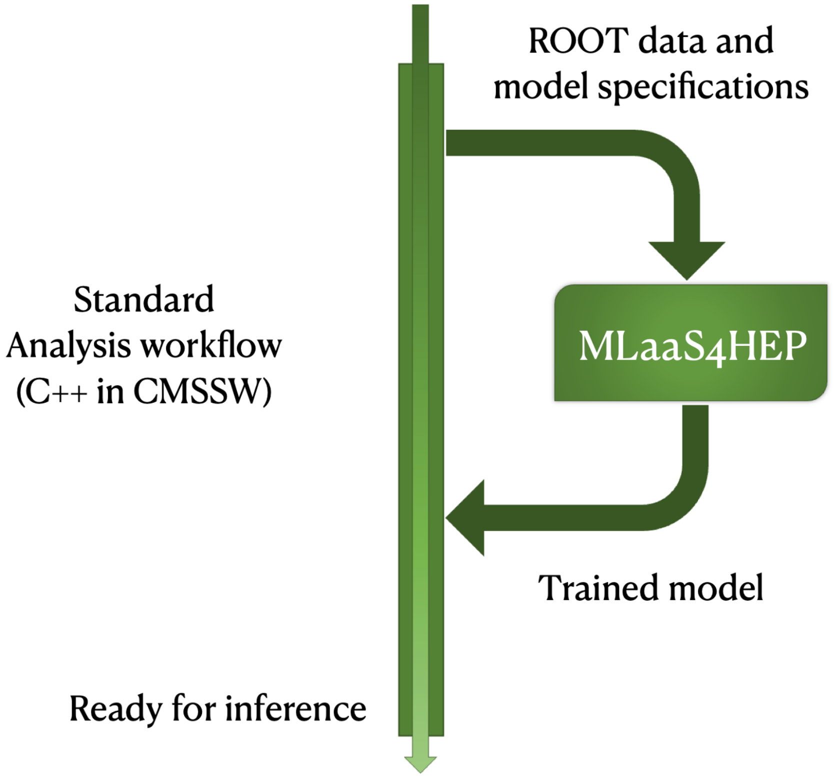
Why Machine Learning as a Service in HEP?

- ML successfully applied in many areas of HEP and it will play a significant role during the upcoming HL-LHC program at CERN

- Developing a ML project and implementing it for production use requires specific skills and is a highly time-consuming task.
  - It would be helpful to provide HEP physicists who are not experts in ML with a **service** that allows them to exploit the potentiality of ML easily

- **MLaaS** solutions offered by major service providers have many services and cover different use cases but are not directly usable in HEP.
  - ROOT data format cannot be directly used
  - Flattening of data from the dynamic size event-based tree format to the fixed-size data representation does not exist
  - Pre-processing operations may be more complex than the ones offered

- There are various **R&D activities underway within HEP** aimed at providing HEP analysts with tools or services to accomplish ML tasks.
  - Solutions designed only for optimization of the inference phase (e.g. hls4ml, SonicCMS)
  - Custom solutions adopted in specific CMS analyses cannot easily generalized and do not represent ''as a Service'' solutions
  - And others…



MLaaS4HEP

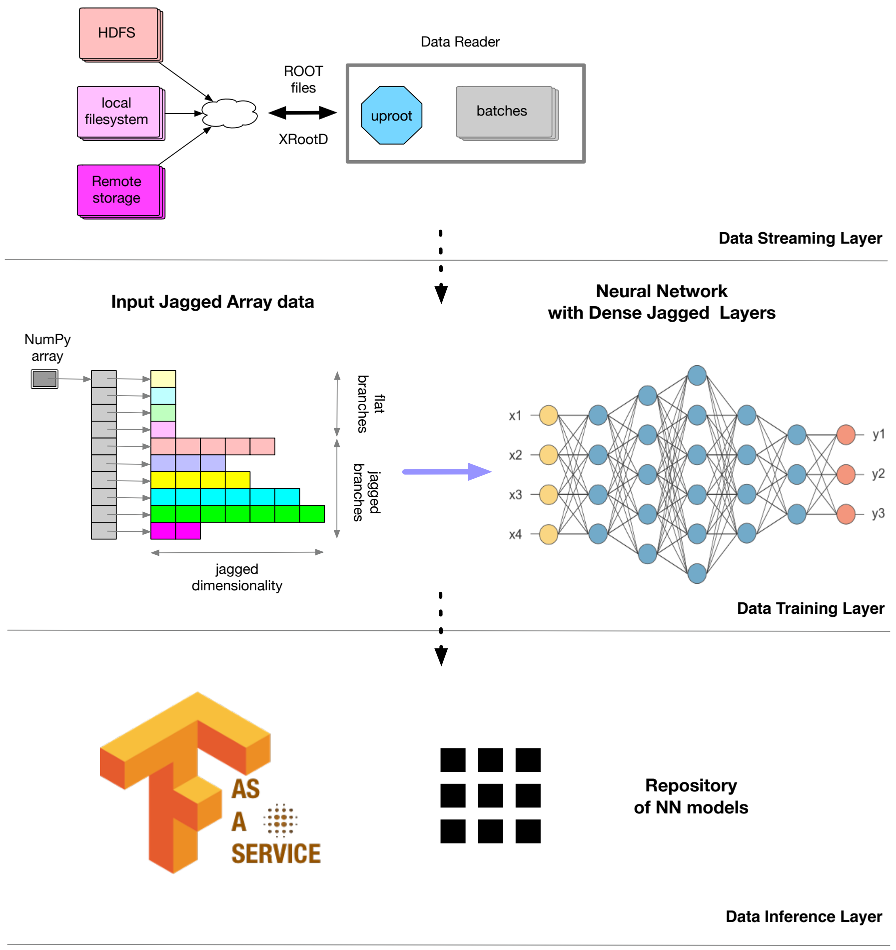
The **MLaaS4HEP** solution aims to:

- ➢ provide transparent access to HEP datasets stored in ROOT files
- ➢ use heterogeneous resources in HEP for training and inference
- ➢ use different ML frameworks of interest in HEP
- ➢ serve pre-trained HEP models and access it easily

MLaaS4HEP framework

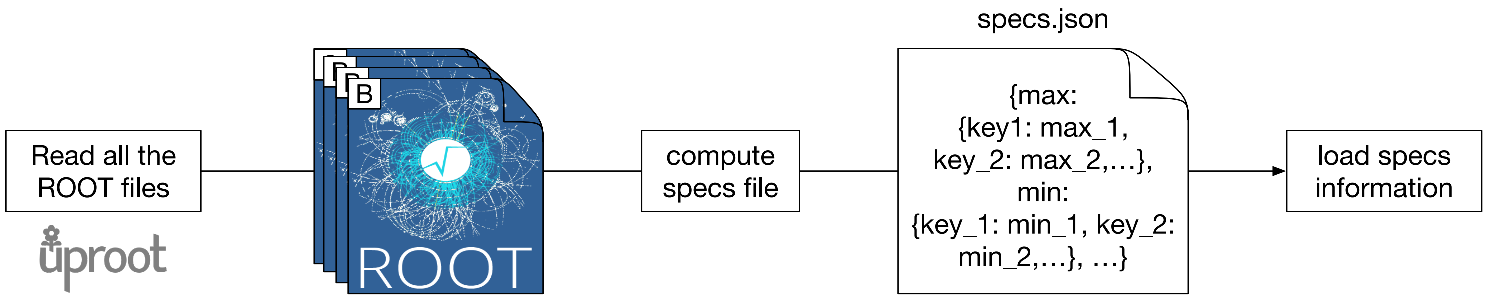
Multi-language architecture: Python and Go

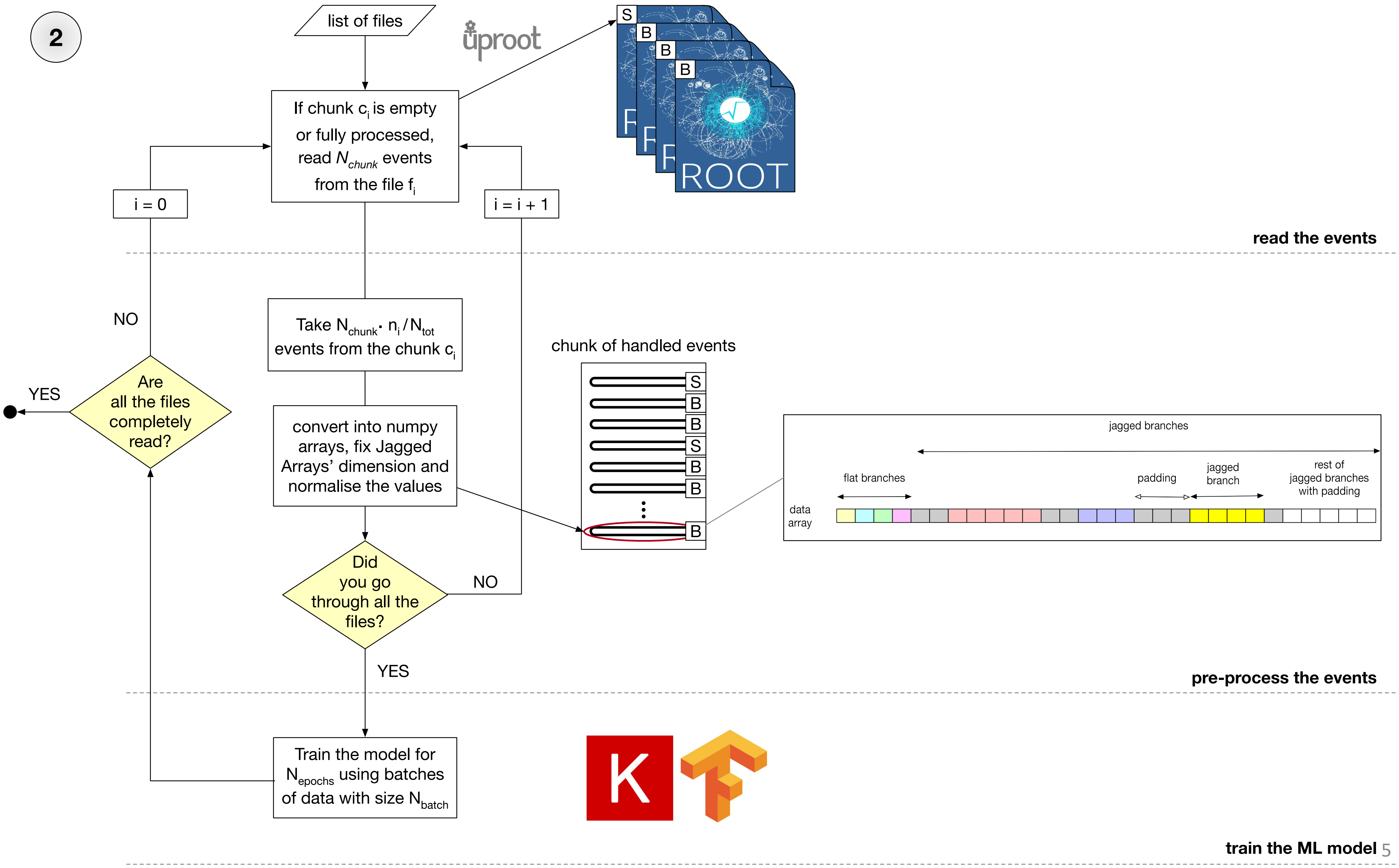
- ➢ **Data Streaming Layer**
  - ○ developed using the Uproot library
  - ○ allows to read ROOT data from local and remote data storage
  - ○ use a Generator to read data in chunks
- ➢ **Data Training Layer**
  - ○ process input data
  - ○ provide a proper normalisation of each attribute
  - ○ use data to train ML model chosen by user
- ➢ **Data Inference Layer**
  - ○ implemented as Tensorflow as a Service (TFaaS)
  - ○ provides access to pre-trained HEP models for inference purpose



Specs computing phase

1





2
list of files
uproot
If chunk c_i is empty or fully processed, read N_{chunk} events from the file f_i
i = 0
i = i + 1
S
B
B
B
ROOT
read the events
NO
Take $N_{chunk} \cdot n_i / N_{tot}$ events from the chunk c_i
chunk of handled events
YES
Are all the files completely read?
convert into numpy arrays, fix Jagged Arrays' dimension and normalise the values
jagged branches
flat branches
padding
jagged branch
rest of jagged branches with padding
data array
Did you go through all the files?
NO
YES
pre-process the events
Train the model for N_{epochs} using batches of data with size N_{batch}
K
train the ML model

Run a MLaaS4HEP workflow

```
./workflow.py --files=files.txt --labels=labels.txt --model=model.py --params=params.json --preproc=preproc.json
```

- MLaaS4HEP training workflow
- Input ROOT files
- Labels related to ROOT files content
- Definition of the ML model
- MLaaS4HEP parameters
- Definition of preprocessing operations (Optional)

Keras model (model.py)

```
from tensorflow import keras
from keras.models import Sequential
from keras.layers import Dense, Dropout

def model(idim):
    "Simple Keras model for testing purposes"
    ml_model = Sequential([Dense(128,
activation='relu',input_shape=(idim,)),
                              Dropout(0.5),
                              Dense(64, activation='relu'),
                              Dropout(0.5),
                              Dense(1, activation='sigmoid')])
    ml_model.compile(optimizer=keras.optimizers.Adam(lr=1e-3),
                     loss=keras.losses.BinaryCrossentropy(),
                     keras.metrics.AUC(name='auc')])
```

MLaaS parameters (params.json)

```
{
    "nevts": 3000,
    "shuffle": true,
    "chunk_size": 1000,
    "epochs": 3,
    "batch_size": 100,
    "identifier": "",
    "branch": "boostedAk8/events",
    "selected_branches":"",
    "exclude_branches": "",
    "hist": "pdfs",
    "redirector": "root://xrootd.ba.infn.it",
    "verbose": 1
  }
```

Input ROOT files (files.txt)

```
PATH/flatTree_ttHJetTobb_M125_13TeV_amcatnloFXFX_madspin_pythia8.root
PATH/flatTree_TT_TuneCUETP8M2T4_13TeV-powheg-pythia8.root
```

Labels of ROOT files (labels.txt)

```
1
0
```

The MLaaS4HEP framework and its developments

1. It is developed to accept **flat ROOT ntuples** (e.g. NANOAOD) as input for **HEP classification problems**

2. It is **ML framework and model agnostic**. Currently, it has been tested using:
   - MLP written in Keras and PyTorch
   - MLP, Gradient Boosting, AdaBoost, Random Forest, Decision Tree, kNN, SVM, and Logistic Regression written in Scikit-learn
   - Gradient Boosting written in XGBoost

3. It is **experiment agnostic**
   - It has been validated, and its performance tested, choosing a signal vs background discrimination problem in a $t\bar{t}H$ analysis of CMS
   - It has been used to tackle the Higgs Boson ML challenge (ATLAS open data)

Developments made

1. It has been updated to support **Uproot4**, enabling **pre-processing operations** defined by the user

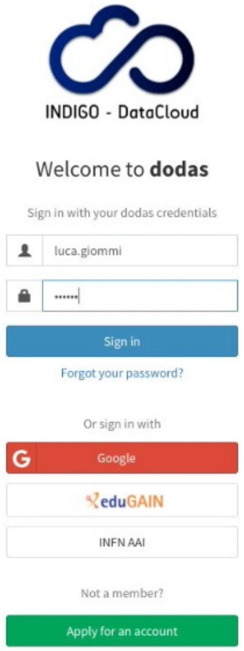
2. **An additional training procedure** of the ML models has been introduced

3. A **SaaS** solution has been provided using **Dynamic On Demand Analysis Service (DODAS)**

SaaS solution for MLaaS4HEP

- A **SaaS** solution for a sharable jupyter notebook has been provided
- Token-based access to the jupyterhub, with the support for a customizable environment

felixfelicislp/mlaas_cloud:mlaas_jupyterhub



- Integrate cloud storage for managing the required files (ROOT files, ML model, etc.)


```
# . ./shared/setup_local
(base) # cd /workarea/shared/folder_test
(base) # ../../workarea/MLaaS4HEP/src/python/MLaaS4HEP/workflow.py --files=files_test.txt --labels=labels_test.txt --model=keras_model.py --params=params_test.json
model parameters: {"nevts": -1, "shuffle": true, "chunk_size": 10000, "epochs": 5, "batch_size": 100, "identifier": ["runNo", "evtNo", "lumi"], "branch": "events",
"selected_branches": "", "exclude_branches": "", "hist": "pdfs", "redirector": "root://gridftp-storm-t3.cr.cnaf.infn.it:1095", "verbose": 1}
Reading ttH_signal.root
# 10000 entries, 29 branches, 1.10626220703125 MB, 0.034181833267211914 sec, 32.364039645948566 MB/sec, 292.5530623775014 kHz
# 10000 entries, 29 branches, 1.10626220703125 MB, 0.022344589233398438 sec, 49.50917626973965 MB/sec, 447.53563807084936 kHz
```

Create a cloud native solution for MLaaS4HEP

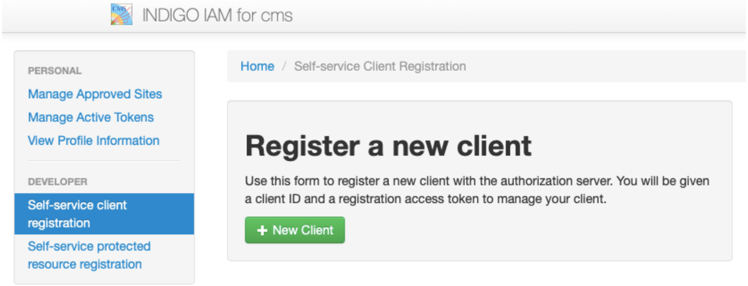
The goal is to create a **cloud service** that could use cloud resources and could be added into the INFN Cloud portfolio of services

- MLaaS4HEP is not yet a service and should be developed as a **cloud native application**. The needed steps are:
  - Provide **APIs** through which a user can interact with it
  - Develop interconnected **microservices**, each of them in charge of different tasks
  - **Containerize** each microservice

- The following microservices have been identified as the **pillars** of the entire MLaaS4HEP service:
  - a **MLaaS4HEP server**, which allows to submit MLaaS4HEP workflow requests and manage all the actions related to it
  - an **authentication/authorization layer**, which allows to authenticate the users and authorize their requests to the MLaaS4HEP server
  - an **XRootD Proxy server**, which allows to use X.509 proxies for the remote access of data

Integrated services

- **MLaaS4HEP server**
  - Written using the (Python-based) Flask framework
- **OAuth2 Proxy server**
  - Register the client with the authorization server: https://cms-auth.web.cern.ch/
  - Use a proper configuration file for the proxy
  - Obtain a token for the registered client using oidc-agent
- **XRootD Proxy server**
  - It creates an X.509 proxy and renews it when it is expired
- **TFaaS**



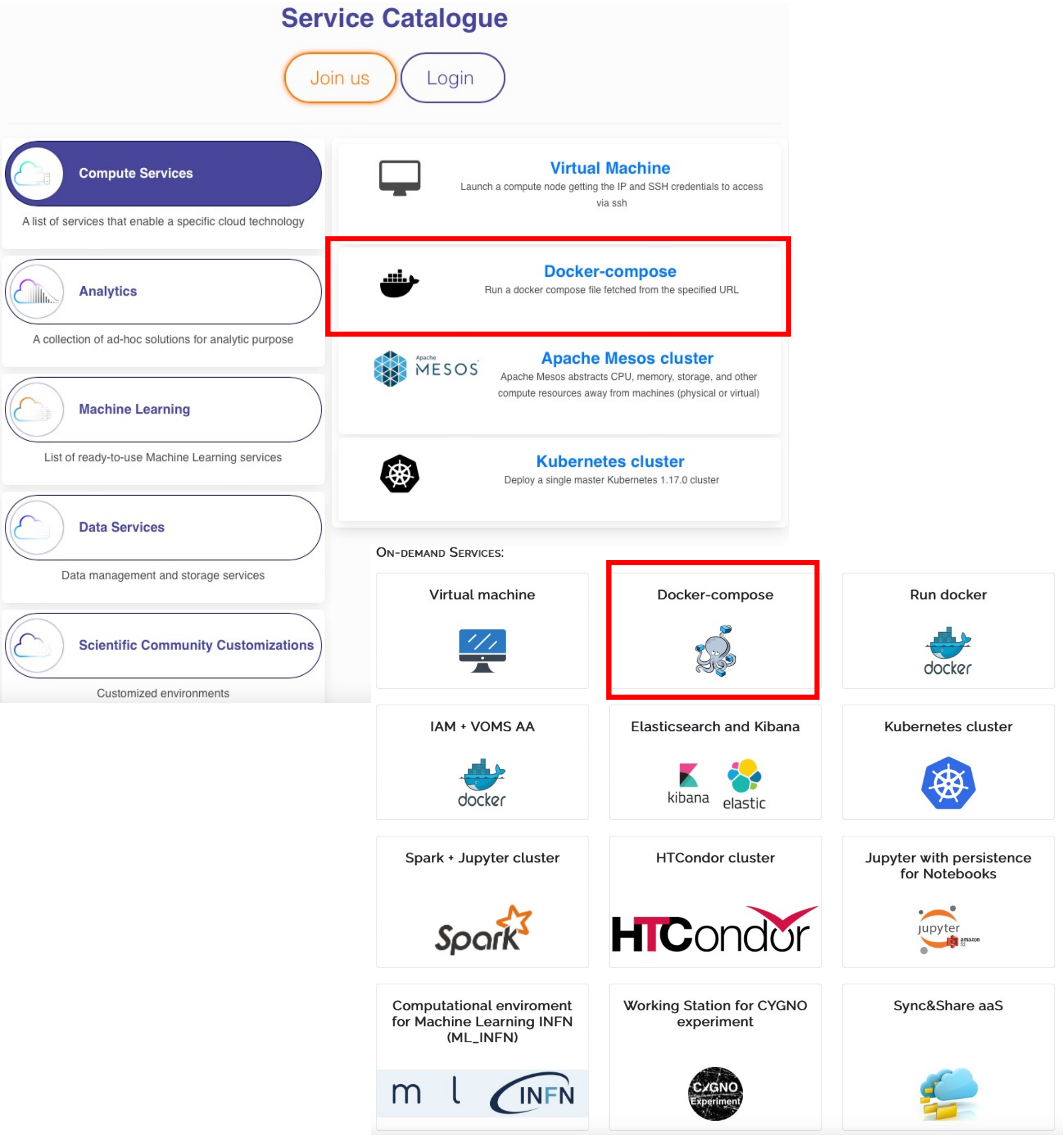
A working prototype of the service is running on a VM of INFN Cloud. Once the user obtains an access token from the authorization server, he/she can contact the MLaaS4HEP server or TFaaS using curl, e.g. in the following ways:

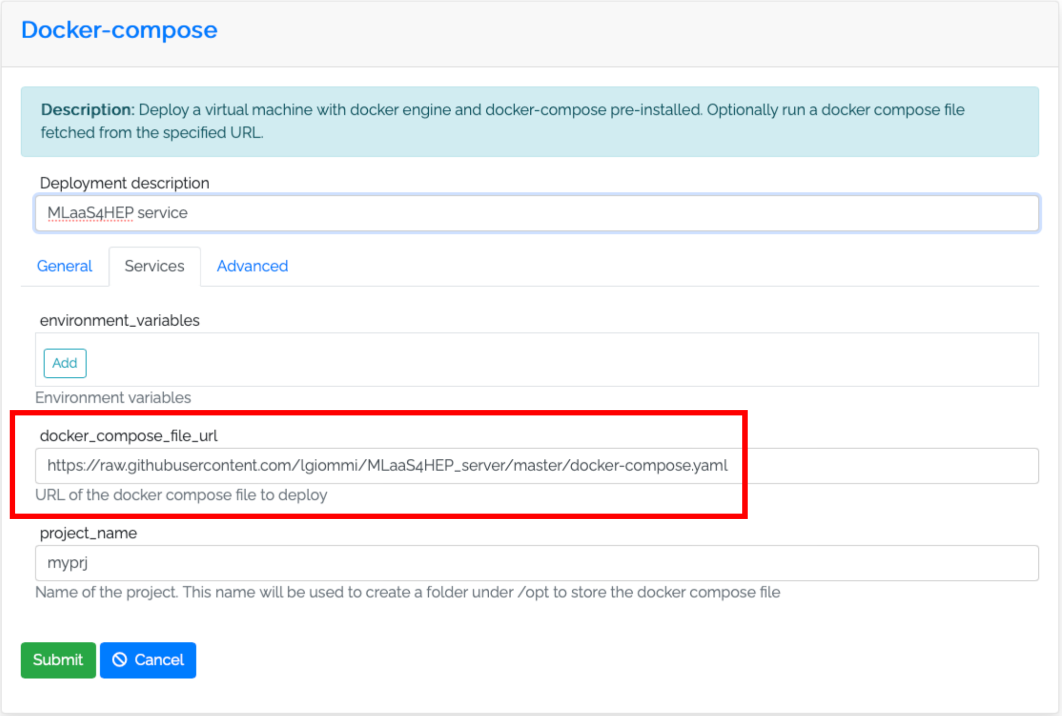
```
curl -L -k -H "Authorization: Bearer ${TOKEN_MLAAS}" -H "Content-Type: application/json" -d @submit.json https://90.147.174.27:4433/submit

curl -L -k -H "Authorization: Bearer ${TOKEN_TFAAS}" -X POST -H "Content-type: application/json" -d @predict_bkg.json https://90.147.174.27:8081/json
```

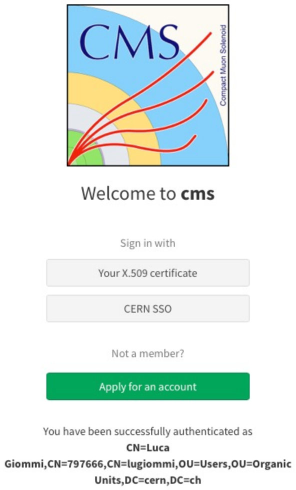
Configuration file for the OAuth2 Proxy server

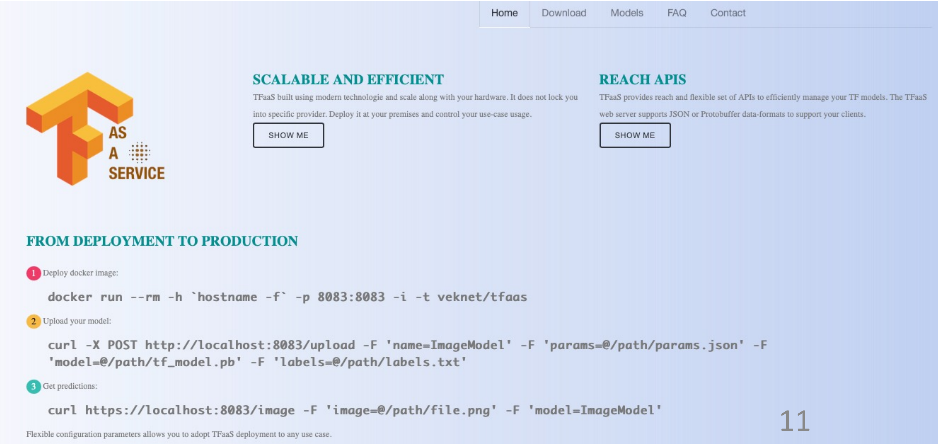
```
provider="oidc"
https_address = ":4433"
redirect_url =
"https://90.147.174.27:4433/oauth2/callback"
oidc_issuer_url = https://cms-auth.web.cern.ch/
upstreams = [ "http://127.0.0.1:8080/" ]
email_domains = [ "*" ]
client_id = "CLIENT_ID"
client_secret = "CLIENT_SECRET"
cookie_secret = "COOKIE_SECRET"
tls_cert_file = "./localhost.crt"
tls_key_file = "./localhost.key"
```

MLaaS4HEP service in INFN Cloud









Conclusions

- The MLaaS4HEP framework allows to perform ML pipelines (read data, pre-process data, train ML models) in HEP while TFaaS can be used for the inference phase
- A working prototype of the MLaaS4HEP service has been deployed on a VM of INFN Cloud
- A **docker compose** file has been developed to deploy the various microservices
- The MLaaS4HEP service deployment can be fully automated using the docker compose deployment of INFN Cloud
- Code available in GitHub (MLaaS4HEP framework, MLaaS4HEP service), MLaaS4HEP service demo available

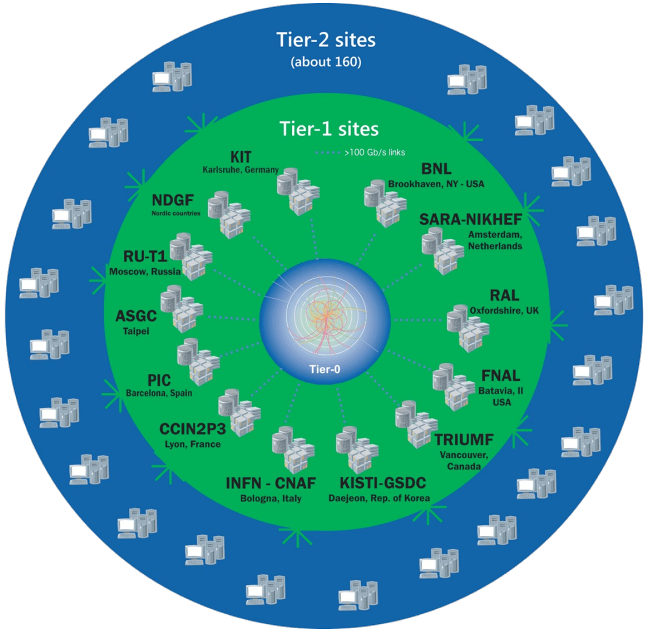
Outlook

- Involve parallelization of I/O, distributed ML training, etc.
- Make MLaaS4HEP usable also for other tasks, e.g. regression problems, image classifications, as well as accept other data formats as input
- Provide a general inference service

Thanks for the attention
Questions?

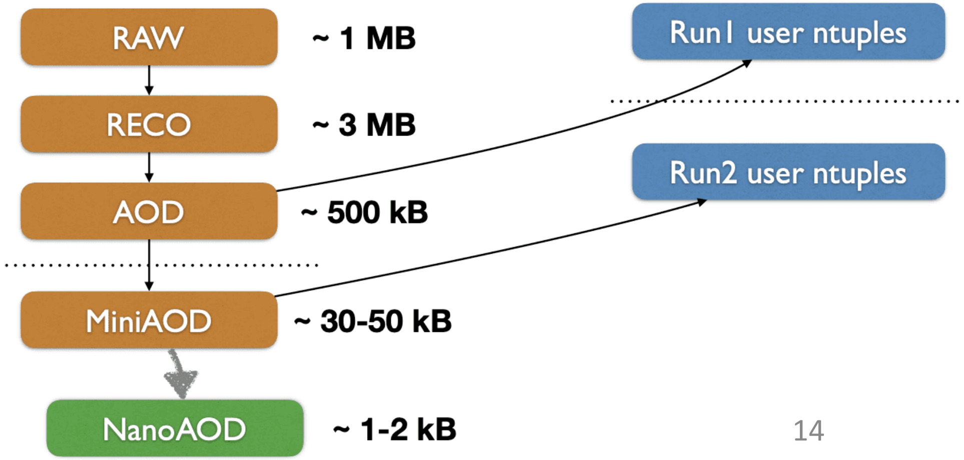
Computing at the Large Hadron Collider

- Collectively, LHC experiments operations produce ~200 PB of data each year that must be stored, processed, and analyzed (the entire amount is ~1.5 EB). To allow physicists to have access to computing power and storage needed to conduct research activities, CERN exploits the **Worldwide LHC Computing Grid (WLCG).**



- Challenges towards **High Luminosity LHC (HL-LHC)**
  - Fitting within the limited budget for computing
  - Managing Exabyte scale data
  - Heterogeneous computing and portability

The **ROOT** framework provides the data format commonly used to store HEP data, as well as tools to access and analyze such data

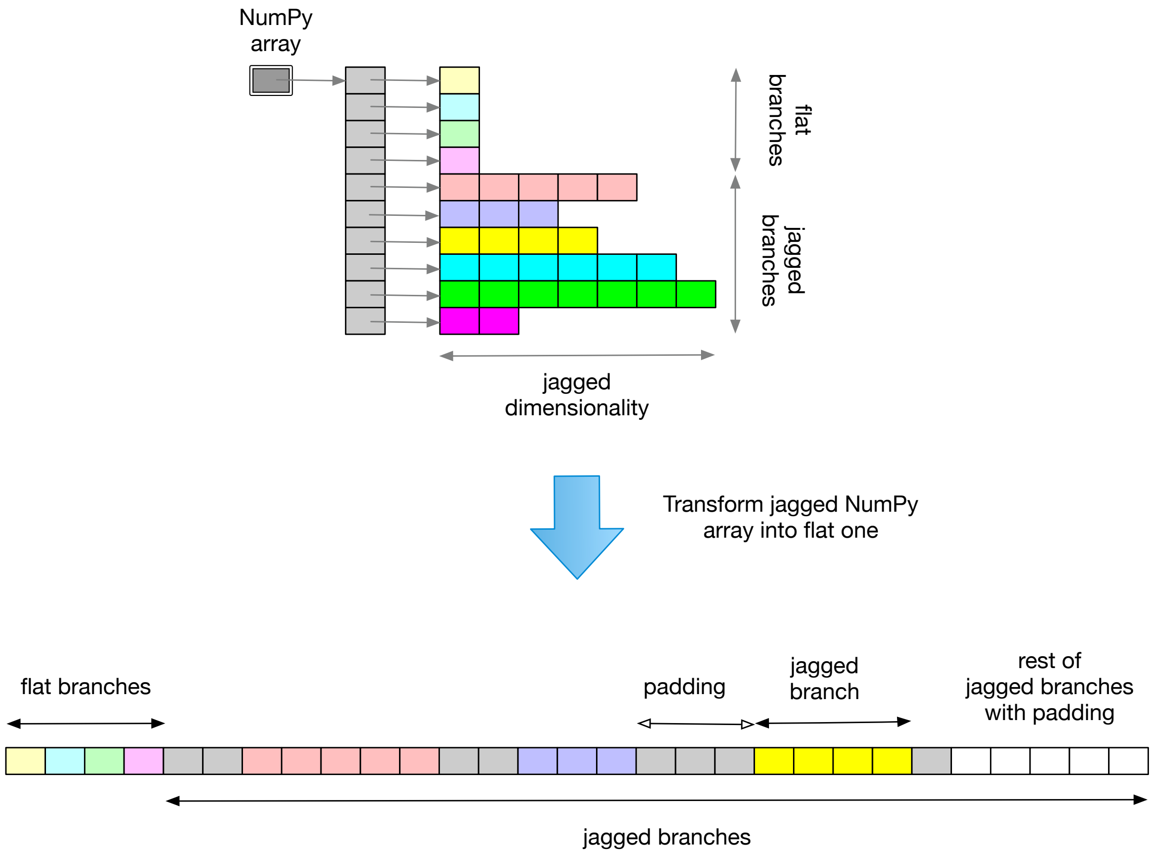


Jagged/Awkward Arrays

- Each event is a composition of flat and **Jagged/Awkward branches**.
    - Jagged Array is a compact representation of variable size event data produced in HEP experiments
    - Such a data representation is not directly suitable for ML

- To feed these data into ML frameworks, the Jagged Arrays are flattened into fixed-size arrays with padding values through a two-step procedure:
    - compute the dimensionality of every Jagged Array attribute
    - update the dimension of the Jagged branches using padding values

- The mask array with padding values location is stored.

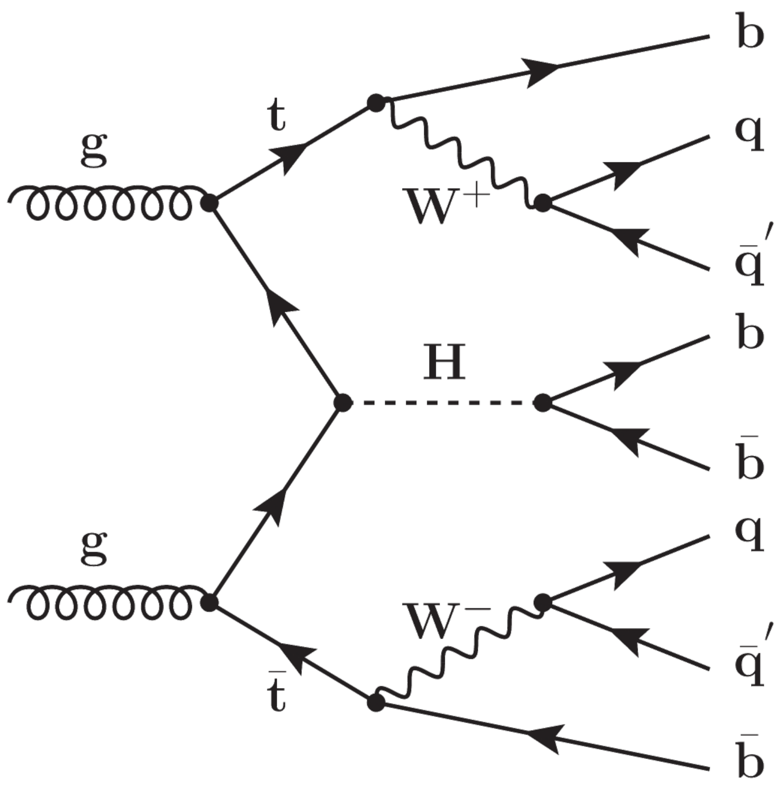


Real case scenario: $t\bar{t}H(bb)$ analysis in the boosted, all-hadronic final states

The MLaaS4HEP framework was tested on a **real physics use-case**: a signal vs background discrimination problem in a $t\bar{t}H$ (CMS) analysis. This allowed to:

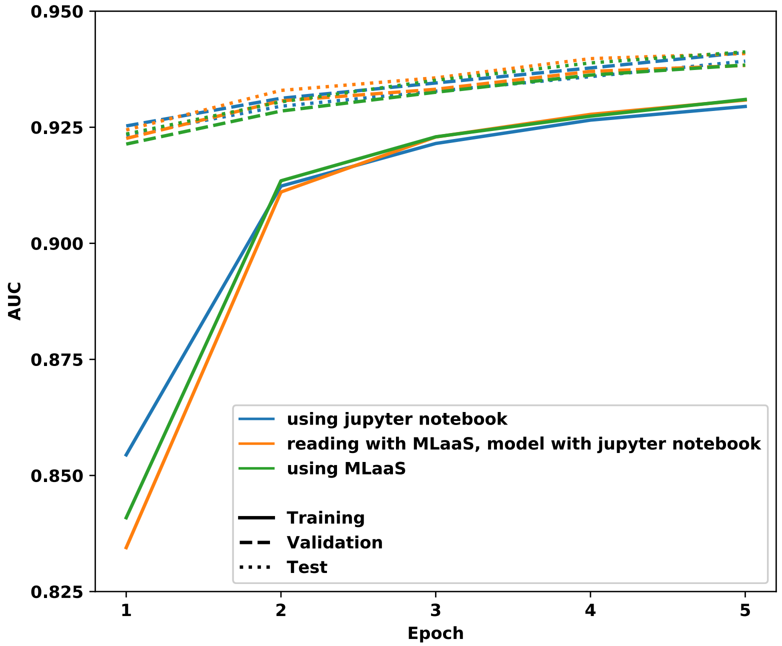
1. **validate** MLaaS4HEP results from the physics point of view
2. **test performances** of MLaaS4HEP framework

For the validation phase 9 ROOT files were used, 8 of background and 1 of signal. Each file has 27 branches, with ~350 thousand events for the whole pool of files and a total size of ~28 MB. The ratio between signal and background is ~10.8%.

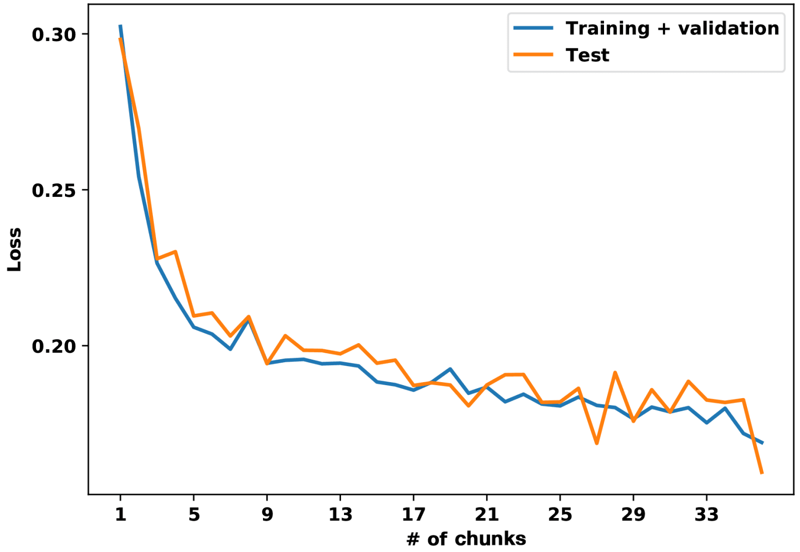


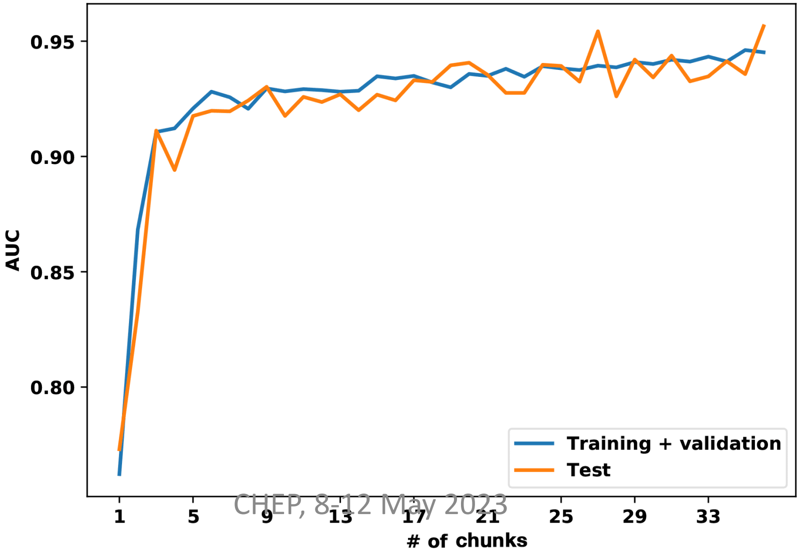
MLaaS4HEP validation

- Validate the MLaaS4HEP approach by comparing it with alternative methods on the reference use-case.
  - A simple NN with Keras in all methods has been chosen
- **Validation successful**: physics results are not impacted.
- The AUC score is also comparable with the BDT-based analysis, performed within the TMVA framework by a subgroup of the CMS HIG PAG.



Chunk size set to the total number of events





Chunk size set to 10k events

Pre-processing operations

- The MLaaS4HEP code has been updated to support **Uproot4** and to allow users to perform **pre-processing operations** on the input ROOT data.

- The migration to the updated version of Uproot allowed to create new branches and to apply cuts, both on new and on existing branches.

```
{
 "new_branch": {

    "log_partonE": {
       "def": "log(partonE)",
       "type": "jagged",
       "cut_1": ["log_partonE<6.31", "any"],
       "cut_2": ["log_partonE>5.85", "all"],
       "remove": "False",
       "keys_to_remove": ["partonE"]},

    "nJets_square": {
       "def": "nJets**2",
       "type": "flat",
       "cut": "1<=nJets_square<=16",
       "remove": "False",
       "keys_to_remove": ["nJets"]}},

 "flat_cut": {
    "nLeptons": {
    "cut": "0<=nLeptons<=2",
    "remove": "False"}},

 "jagged_cut": {
    "partonPt": {
    "cut": ["partonPt>200", "all"],
    "remove": "False"}}}
```

MLaaS4HEP performance

- In the phase of **testing the MLaaS4HEP performance**, all available ROOT files without any physics cut were used. This gave a dataset with ~28.5M events with 74 branches (22 flat and 52 Jagged), and a total size of ~10.1 GB.

- All the tests were performed running the MLaaS4HEP framework on:
  - macOS, 2.2 GHz Intel Core i7 dual-core, 8 GB of RAM
  - CentOS 7 Linux, 4 VCPU Intel Core Processor Haswell 2.4 GHz, 7.3 GB of RAM CERN Virtual Machine

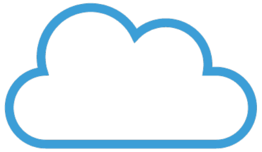
- The ROOT files are read from **local** file-systems (SSD storages) and remotely from the **Grid sites,** stored in three different data-centers located at Bologna (BO), Pisa (PI), Bari (BA).

- Based on the resource used and if the ROOT files were local or remote, the results obtained are:
  - **specs computing phase** (chunk size = 100k events)
    - Event throughput: **8.4k – 13.7k evts/s**
    - Total time using all the 28.5M events: 35 – 57 min
  - **chunks creation in the training phase** (chunk size = 100k events)
    - Event throughput: **1.1k – 1.2k evts/s**
    - Total time using all the 28.5M events: 6.5 – 7.5 hrs

- In the reading phase there is a worse performance using Uproot4 than using Uproot3 but in the chunk creation phase, there is better performance with Uproot4.
  - Strong performance degradation when cuts on existing Jagged branches and on new branches are applied

Towards MLaaS4HEP cloudification

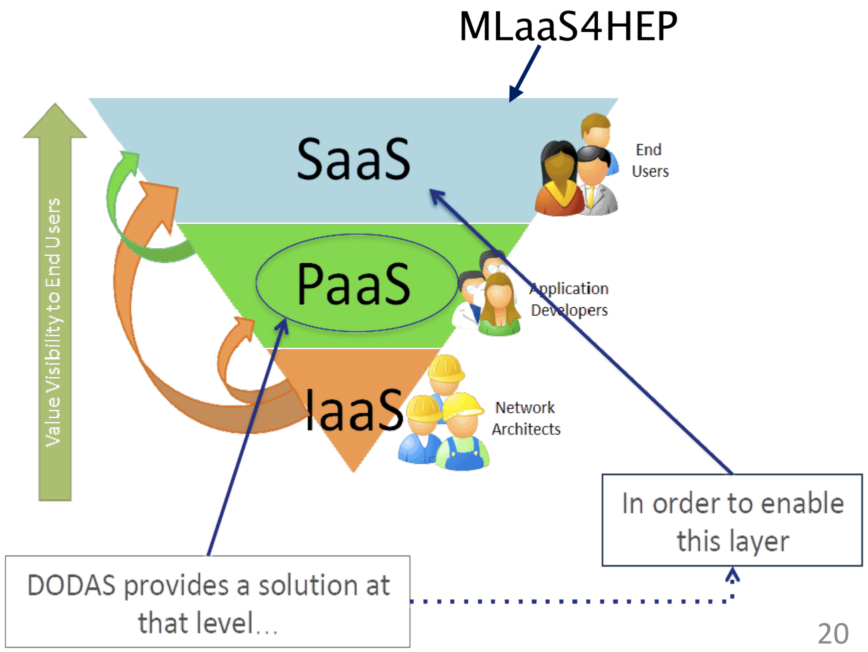
- The MLaaS4HEP performance strictly depends on the available hardware resources. How to **improve** it?
  - Adopt new solutions in the code
  - Invest in better and more expensive on-premise resources
  - Move to the cloud



- The operation of **cloudification** has two benefits.
  - Opens to potentially more performing resources
  - Opens to the creation of an ''as a Service'' solution

- Work towards the MLaaS4HEP cloudification using **DODAS**

Dynamic On Demand Analysis Service (DODAS) is a Platform as a Service tool for generating over cloud resources and on-demand, container based solution.



MLaaS4HEP cloudification with DODAS

Creation of a docker image able to run the workflow.py script

Create an Ansible playbook to automatize the configuration and deployment of the container with dependencies

Convert the Ansible playbook into an Ansible role

Creation of a Tosca template to define the resource requirements and the input parameters for the creation of the docker container

Create the deployment from command line

Run workflow.py interactively or with jupyterhub

```
dodas create lgiommi-template.yml
dodas login <infID> <vmID>
```

MLaaS parameters

Read remote ROOT files
and compute specs

Write and load the specs

```
./workflow.py --files=files.txt --labels=labels.txt —model=model.py --params=params.json
DataGenerator: <MLaaS4HEP.generator.RootDataGenerator object at 0x7f0cb58d7fd0> [29/Jun/2020:17:53:[illegible]] 1593445994.0
model parameters: {"nevts": 30000, "shuffle": true, "chunk_size": 10000, "epochs": 2, "batch_size": 100, "identifier":
["runNo", "evtNo", "lumi"], "branch": "boosted[illegible]8/events", "selected_branches": "", "exclude_branches": "", "hist": "pdfs",
"redirector": "root://xrootd.ba.infn.it", "verbose": 1}


Reading root://xrootd.ba.infn.it//store/user/lgiommi/ttHJetTobb_M125_13TeV_amcatnloFXFX_madspin_pythia8.root
# 10000 entries, 77 branches, 9.52220344543[illegible]7 MB, 1.0169336795806885 sec, 9.36364252323795 MB/sec, 9.833482950553169 kHz
# 10000 entries, 77 branches, 9.53391551971[illegible]355 MB, 1.2977769374847412 sec, 7.346343770133804 MB/sec, 7.705484441248654 kHz
# 10000 entries, 77 branches, 9.53866767887[illegible]008 MB, 1.4104814529418945 sec, 6.7627033726234735 MB/sec, 7.089777734505208 kHz
--- first pass: 948348 events, (22-flat, 5[illegible]-jagged) branches, 328 attrs
<MLaaS4HEP.reader.RootDataReader object at 0x7f840dbf4d50> init is complete in 4.852992534637[illegible]1 sec


Reading root://xrootd.ba.infn.it//store/user/lgiommi/TT_TuneCUETP8M2T4_13TeV-powheg-pythia8.root
# 10000 entries, 77 branches, 8.875920295715332 MB, 0.9596493244171143 sec, 9.2491288951894[illegible] MB/sec, 10.42047313071777 kHz
# 10000 entries, 77 branches, 8.868906021118164 MB, 1.2938923835754395 sec, 6.8544386949790[illegible]8 MB/sec, 7.728618026459661 kHz
# 10000 entries, 77 branches, 8.869449615478516 MB, 1.1267895698547363 sec, 7.871433897477[illegible]9 MB/sec, 8.874771534572496 kHz
--- first pass: 1003980 events, (22-flat, 52-jagged) branches, 312 attrs
<MLaaS4HEP.reader.RootDataReader object at 0x7f8410e15f90> init is complete in 4.53512477[illegible]47559 sec


write global-specs.json
load specs from global-specs.json for root://xrootd.ba.infn.it//store/user/lgiommi/ttHJetTobb_M125_13TeV_amcatnloFXFX_madspin_pythia8.root
load specs from global-specs.json for root://xrootd.ba.infn.it//store/user/lgiommi/TT_TuneCUETP8M2T4_13TeV-powheg-pythia8.root
init RootDataGenerator in 11.186564683914185 sec
```

```
label 1, file <ttHJetTobb_M125_13TeV_amcatnloFXFX_madspin_pythia8.root>, going to read 4858 events
read chunk [0:4857] from /store/user/lgiommi/ttHJetTobb_M125_13TeV_amcatnloFXFX_madspin_pythia8.root
# 10000 entries, 77 branches, 9.52220344543457 MB, 1.3816642761230469 sec, 6.891835889507034 MB/sec, 7.237648228164387 kHz
total read 4858 evts from /store/user/lgiommi/ttHJetTobb_M125_13TeV_amcatnloFXFX_madspin_pythia8.root


label 0, file <TT_TuneCUETP8M2T4_13TeV-powheg-pythia8.root>, going to read 5142 events
read chunk [4858:9999] from /store/user/lgiommi/TT_TuneCUETP8M2T4_13TeV-powheg-pythia8.root
# 10000 entries, 77 branches, 8.875920295715332 MB, 1.7170112133026123 sec, 5.169401473297779 MB/sec, [illegible].8240737873606205 kHz
total read 5142 evts from /store/user/lgiommi/TT_TuneCUETP8M2T4_13TeV-powheg-pythia8.root
```

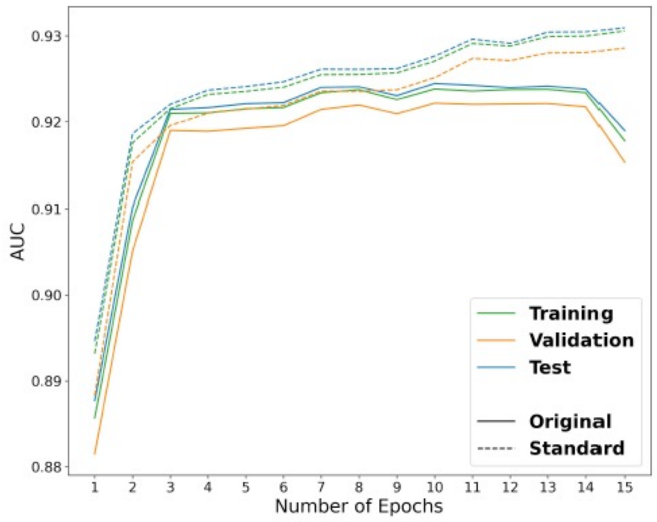
Read events from remote ROOT files,
pre-process them and create the chunk

MLaaS4HEP performance: Uproot3 vs Uproot4

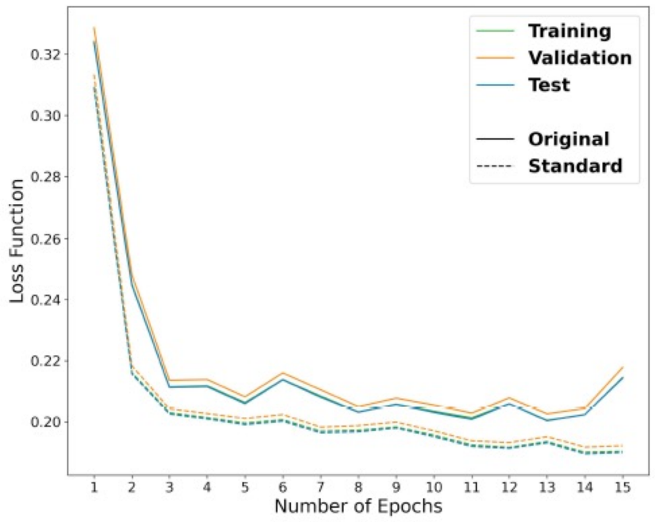
	Uproot3	Uproot4
reading time (s)	1136 (2)	1301 (4)
specs comp. time (s)	653 (1)	607 (1)
time to complete step 1 (s)	1796 (3)	1914 (5)
mean event throughput for reading (evts/s)	25304 (44)	21995 (73)
mean event throughput for specs comp. (evts/s)	43604 (50)	46968 (50)
mean event throughput for reading + specs comp. (evts/s)	16012 (24)	14980 (38)
event throughput for creating a chunk (evts/s)	1197 (5)	1406 (14)

	no cut	flat cut	Jagged cut	new branch cut	mixed cuts
mean event throughput for reading (evts/s)	15157 (71)	15325 (56)	22505 (64)	19718 (51)	19375 (20)
mean event throughput for specs comp. (evts/s)	44004 (52)	43600 (136)	947 (4)	878 (11)	944 (5)
mean event throughput for reading + specs comp. (evts/s)	11273 (37)	11339 (29)	908 (3)	841 (10)	900 (5)
event throughput for creating a chunk (evts/s)	1363 (3)	1395 (8)	125 (1)	124 (1)	124 (1)

Comparison of the two MLaaS4HEP training procedures

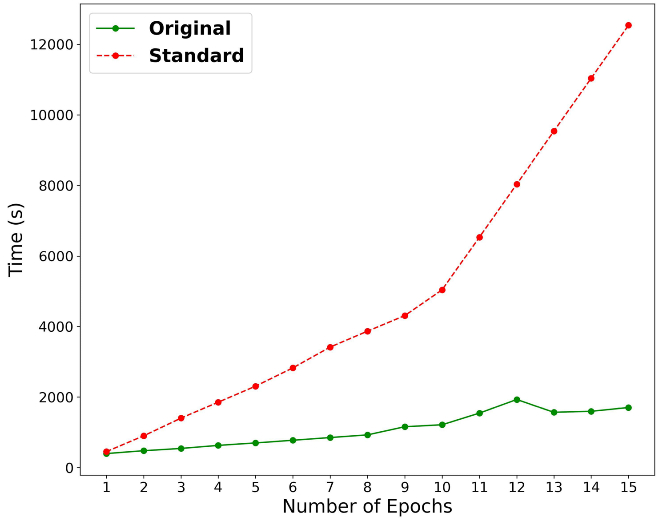


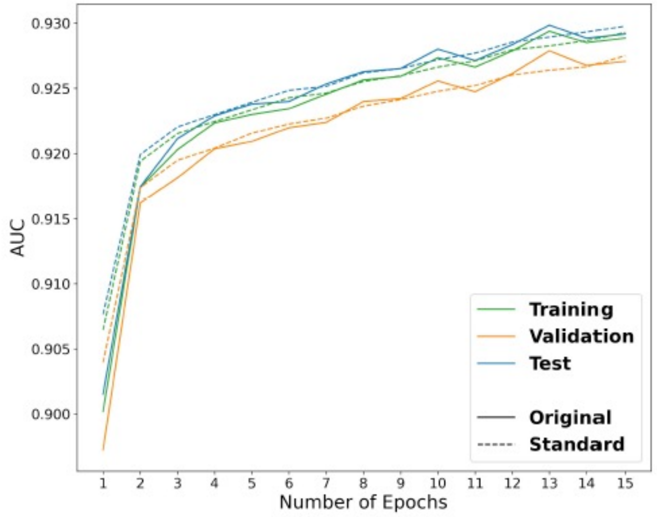
(a)



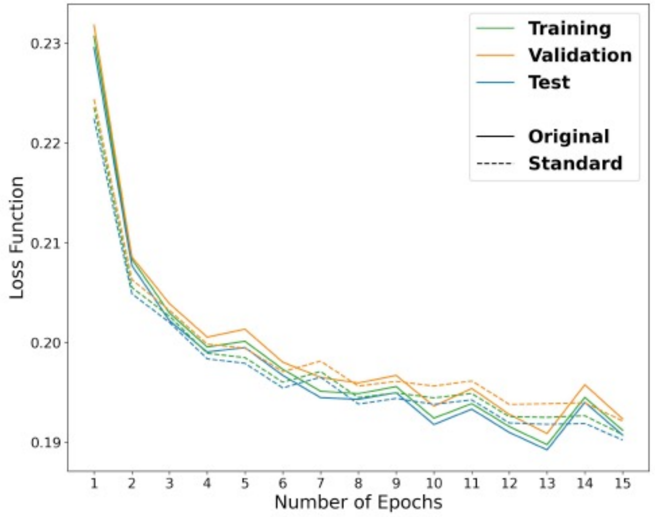
(b)

Chunk size
100 events



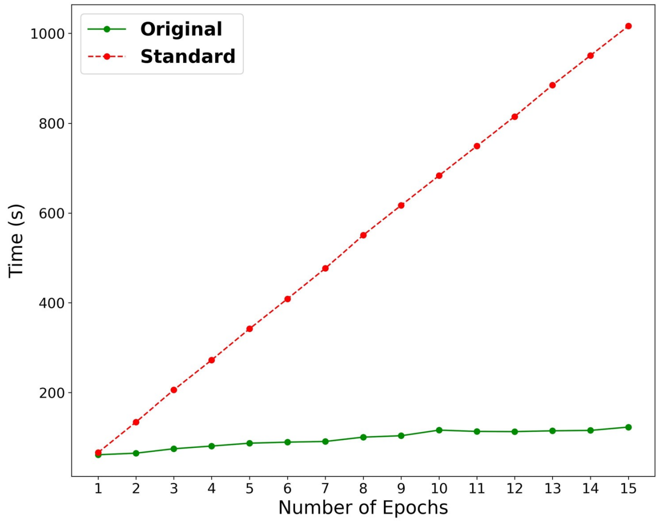


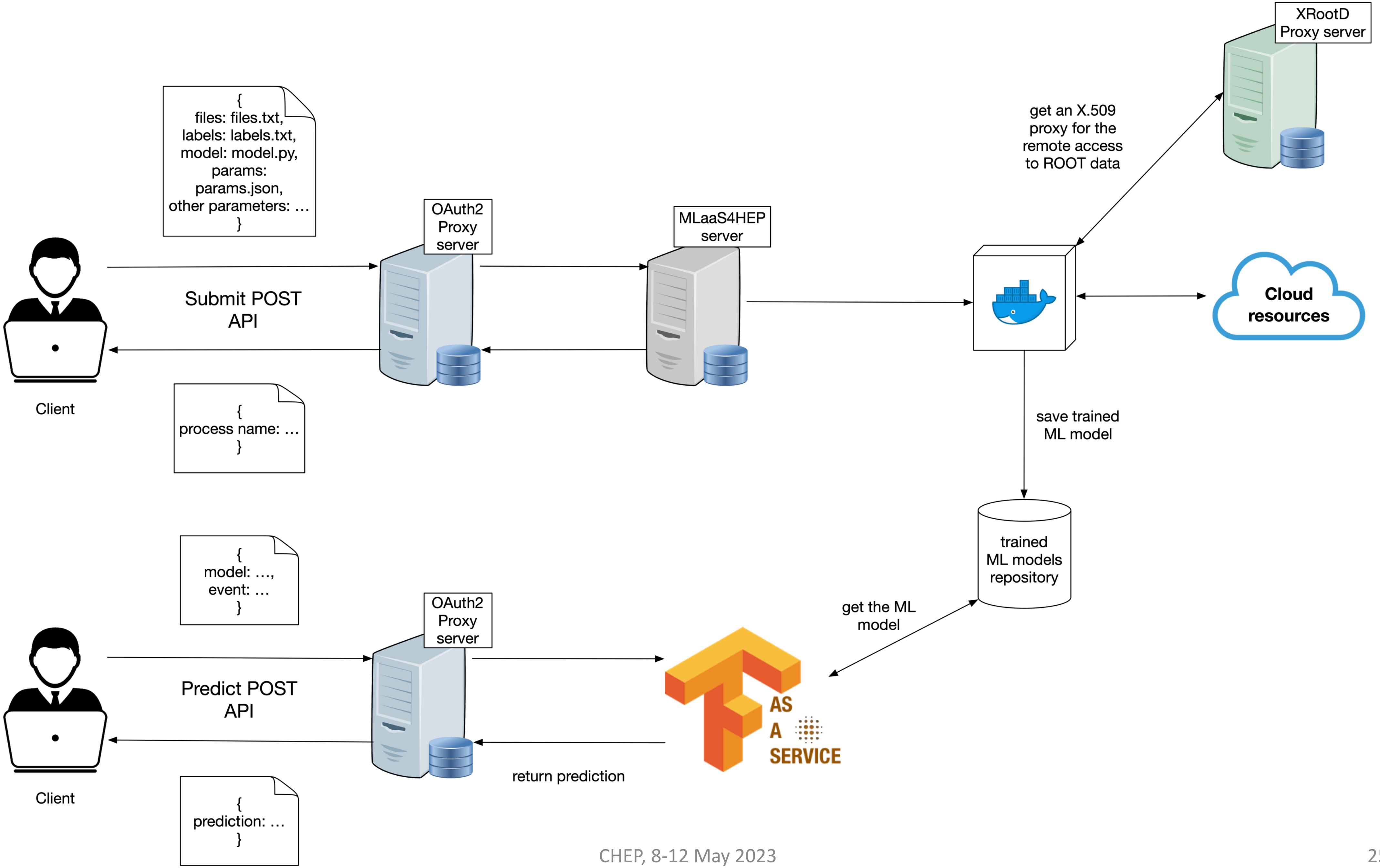
(c)



(d)

Chunk size
100k events




{
files: files.txt,
labels: labels.txt,
model: model.py,
params:
params.json,
other parameters: …
}
OAuth2
Proxy
server
MLaaS4HEP
server
XRootD
Proxy server
get an X.509
proxy for the
remote access
to ROOT data
Submit POST
API
Client
{
process name: …
}
Cloud
resources
save trained
ML model
trained
ML models
repository
{
model: …,
event: …
}
OAuth2
Proxy
server
get the ML
model
Predict POST
API
AS
A
SERVICE
Client
return prediction
{
prediction: …
}