Big Data Tools and Pipelines for Machine Learning in HEP

CERN-EP/IT Data Science Seminar
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Why "Big Data" Ecosystem for HEP?

- Platforms, tools and R&D
  - Large amounts of innovation by open source communities, industry, academia
  - Address key challenges for data intensive domains
  - Lower cost of development and licensing
- Use of mainstream technologies (Data, ML/AI)
  - Create opportunities for collaboration
    - With other sciences (astronomy, biology, etc) + with industry
  - Talent flow: job market for data scientists and data engineers

Data Engineering to Enable Effective ML

- From "Hidden Technical Debt in Machine Learning Systems", D. Sculley at al. (Google), paper at NIPS 2015

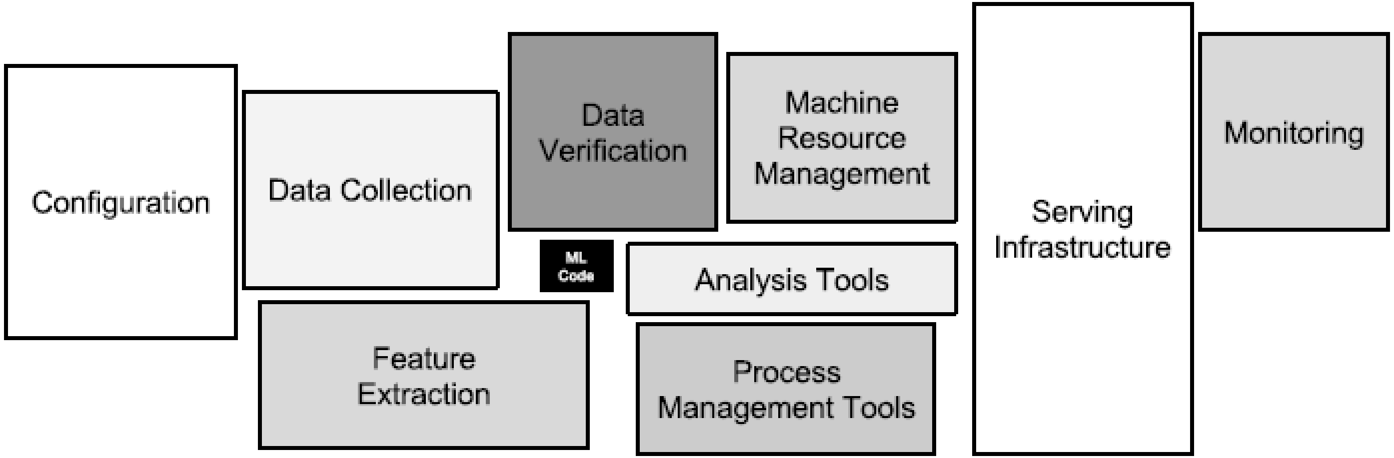
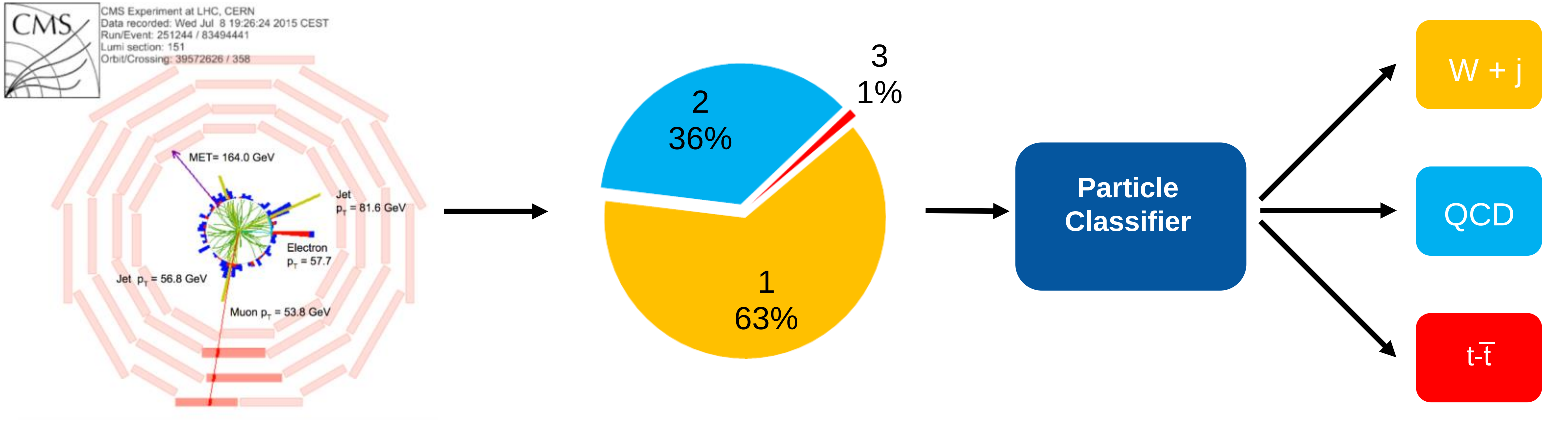


Figure 1: Only a small fraction of real-world ML systems is composed of the ML code, as shown by the small black box in the middle. The required surrounding infrastructure is vast and complex.

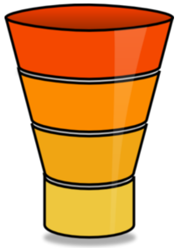
Use Case: End-to-End ML Pipeline

Particles Classifier Using Neural Networks

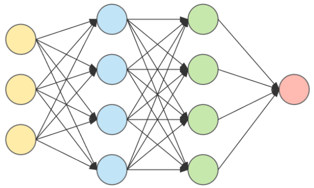
- R&D to improve the **quality of filtering systems**
  - Develop a "Deep Learning classifier" to be used by the filtering system
  - Goal: Identify events of interest for physics and reduce false positives
    - False positives have a cost, as wasted storage bandwidth and computing
  - "Topology classification with deep learning to improve real-time event selection at the LHC", Nguyen et al. **Comput.Softw.Big Sci. 3 (2019) no.1, 12**



R&D – Data Pipelines



- Improve the **quality of filtering systems**
  - Reduce false positive rate
  - Complement or replace rule-based algorithms with classifiers based on Deep Learning



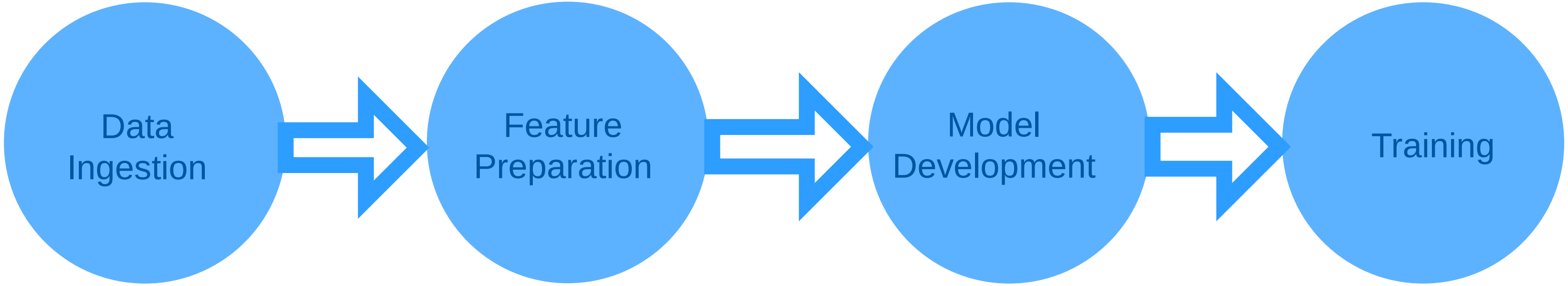
- Advanced analytics **at the edge**
  - Avoid wasting resources in offline computing
  - Reduction of operational costs

Data Flow at LHC Experiments

40 million collisions per second (Raw) → PB/s → 100,000 selections per second (L1) → TB/s → 1,000 selections per second (L2) → GB/s

This can generate up to a petabyte of raw data per second
Reduced to GB/s by filtering in real time
Key is how to select potentially interesting events (trigger systems).

Deep Learning Pipeline for Physics Data



Read physics data and feature engineering

Prepare input for Deep Learning network

1. Specify model topology
2. Tune model topology on small dataset

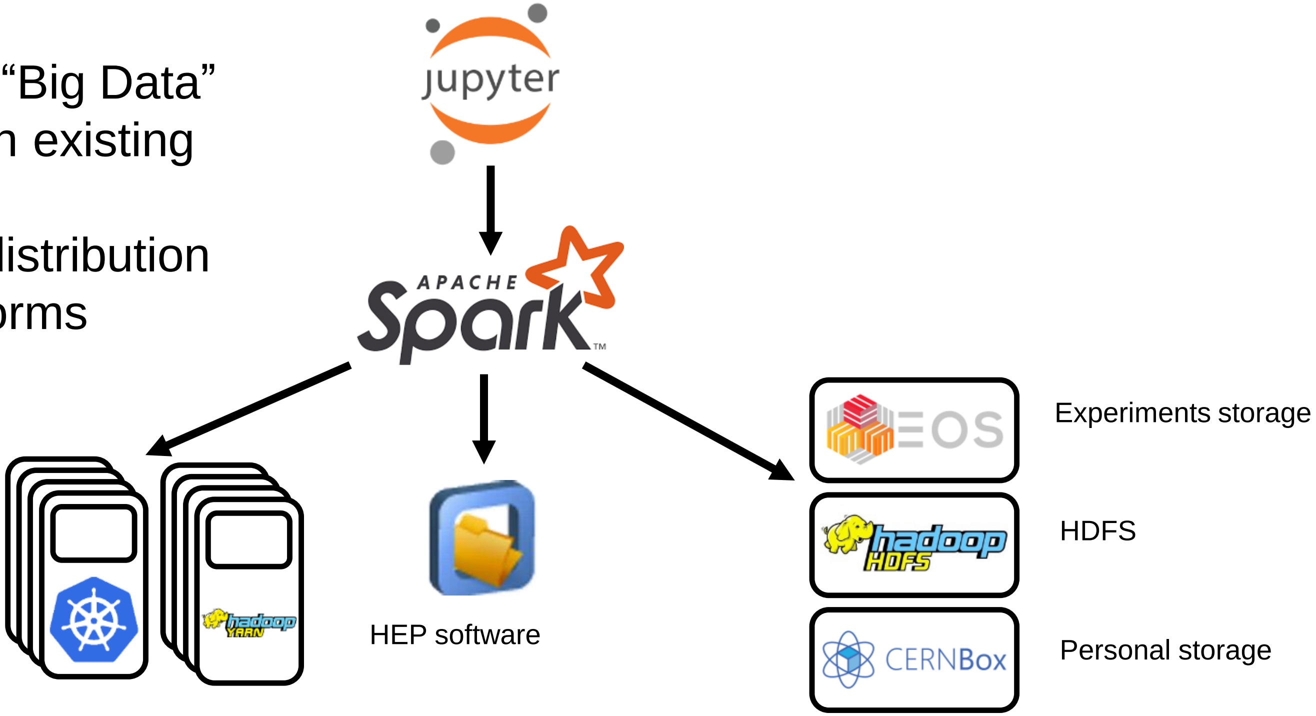
Train the best model

Technology: the pipeline uses Apache Spark + Analytics Zoo and TensorFlow/Keras. Code on Python Notebooks.

CERN SWAN with Apache Spark, a Data Analysis Platform at Scale

Integrating new “Big Data” components with existing infrastructure:

- Software distribution
- Data platforms



FILE EDIT VIEW INSERT CELL KERNEL HELP Trusted Python 2

Do the heavylifting in spark and collect aggregated view to panda DF

In [11]:
```
df_loadAvg_pandas = spark.sql("SELECT submitter_host, \
                              avg(body.LoadAvg) as avg, \
                              hour(from_unixtime(timestamp / 1000, 'yyyy-MM-dd HH:mm:ss')) as hr \
                       FROM loadAvg \
                       WHERE submitter_hostgroup = 'hadoop/itdb/datanode' \
                       AND dayofmonth(from_unixtime(timestamp / 1000, 'yyyy-MM-dd HH:mm:ss')) = 15 \
                       GROUP BY hour(from_unixtime(timestamp / 1000, 'yyyy-MM-dd HH:mm:ss')), submitter_host")\
          .toPandas()
```

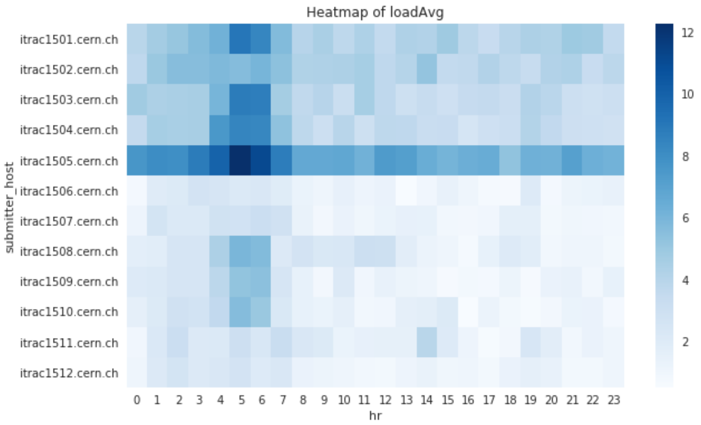
Apache Spark: 90 EXECUTORS 180 CORES Jobs: 1 COMPLETED

Job ID	Job Name	Status	Stages	Tasks	Submission Time	Duration
3	toPandas	COMPLETED	2/2	388 / 388	4 minutes ago	36s

Visualize with seaborn

In [19]:
```
# heatmap of service availability
plt.figure(figsize=(10, 6))
ax = sns.heatmap(df_loadAvg_pandas.pivot(index='submitter_host', columns='hr', values='avg'), cmap="Blues")
ax.set_title("Heatmap of loadAvg")
```

Out[19]: Text(0.5,1,u'Heatmap of loadAvg')



Text

Code

Monitoring

Visualizations

Spark Clusters at CERN: on Hadoop and on Cloud

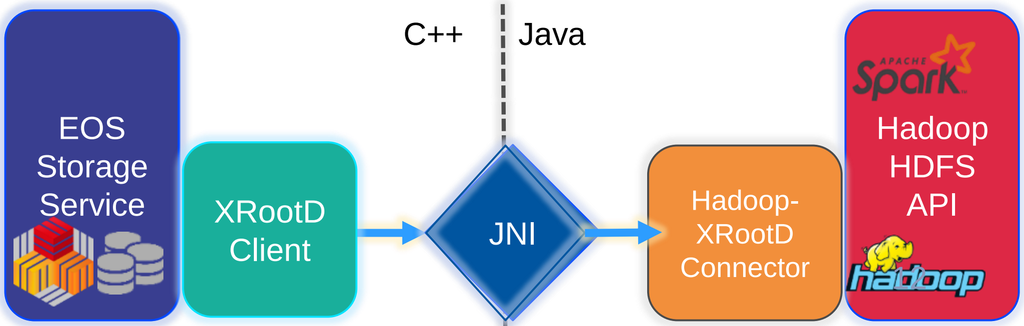
- Clusters run on
  - Hadoop clusters: Spark on YARN
  - Cloud: Spark on Kubernetes
- Hardware: commodity servers, continuous refresh and capacity expansion

NXCals for Accelerator Logging (part of LHC infrastructure)	Hadoop - YARN – 32 nodes (Cores - 1024, Mem - 16 TB, Storage – 7.5 PB)
General Purpose (Analytix + Hadalytic)	Hadoop - YARN, 54 nodes (Cores – 1184, Mem – 21 TB, Storage – 11 PB)
Cloud containers	Kubernetes on Openstack VMs, Cores - 250, Mem – 2 TB Storage: remote HDFS or EOS (for physics data)

Extending Spark to Read Physics Data

- Physics data
  - Currently: >300 PBs of Physics data, increasing ~90 PB/year
  - Stored in the CERN EOS storage system in ROOT Format and accessible via XRootD protocol
- Integration with Spark ecosystem
  - Hadoop-XRootD connector, HDFS compatible filesystem
  - Spark Datasource for ROOT format

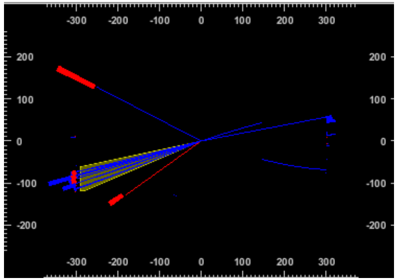
https://github.com/cerndb/hadoop-xrootd
https://github.com/diana-hep/spark-root

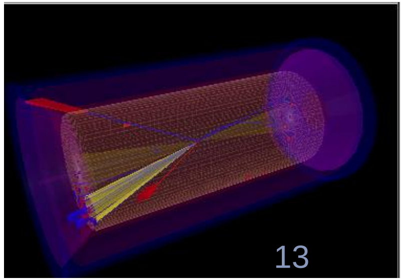


Labeled Data for Training and Test

- Simulated events
  - Software simulators are used to generate events and calculate the detector response
  - Raw data contains arrays of simulated particles and their properties, stored in ROOT format
  - 54 million events

DELPHES
fast simulation

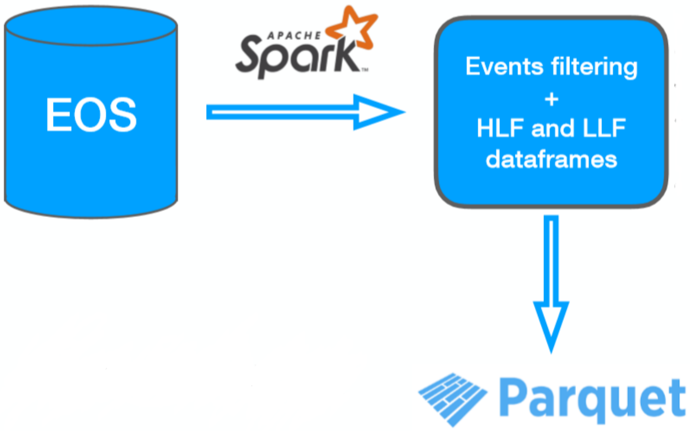




Step 1: Data Ingestion

- Read input files: 4.5 TB from ROOT format
- Feature engineering
  - Python and PySpark code, using Jupyter notebooks
- Write output in Parquet format

Input:
- 54 M events ~4.5 TB
- Physics data storage (EOS)
- Physics data format (ROOT)



Output:
- 25 M events
- 950 GB in Parquet format
- Target storage (HDFS or EOS)

Spark DataFrames – Some Basics

- Data in Apache Spark
  - The key abstraction and API is DataFrame
  - Think of it as “a distributed version of Pandas DF”
- Can parallelize/distribute I/O and operations
  - Large choice of data formats for input and output (extendable)
  - Can do I/O with HDFS, EOS, S3, local filesystem, …
  - Scale out: actions operate in parallel with data partition granularity, run on cluster resources of choice (YARN, K8S, local machine)

```
myDF = spark.read.format("root").load("root://eos….")
myDF.count()
```

Feature Engineering

- Filtering
  - Multiple filters, keep only events of interest
  - Example: “events with one electrons or muon with Pt > 23 Gev”

- Prepare “Low Level Features”
  - Every event is associated to a matrix of particles and features (801x19)

```
features = [
    'Energy', 'Px', 'Py', 'Pz', 'Pt', 'Eta', 'Phi',
    'vtxX', 'vtxY', 'vtxZ', 'ChPFIso', 'GammaPFIso', 'NeuPFIso',
    'isChHad', 'isNeuHad', 'isGamma', 'isEle', 'isMu', 'Charge'
]
```

- High Level Features (HLF)
  - Additional 14 features are computed from low level particle features
  - Calculated based on domain-specific knowledge using Python code

Step 2: Feature Preparation

Features are converted to formats suitable for training

- One Hot Encoding of categories
- MinMax scaler for High Level Features
- Sorting Low Level Features: prepare input for the sequence classifier, using a metric based on physics. This use a Python UDF.
- Undersampling: use the same number of events for each of the three categories

Result

- 3.6 Million events, 317 GB
- Shuffled and split into training and test datasets
- Code: in a Jupyter notebook using PySpark with Spark SQL and ML

Feature preparation

Elements of the `hfeatures` column are list, hence we need to convert them into `Vectors.Dense`

In [10]:
```
from pyspark.ml.linalg import Vectors, VectorUDT
from pyspark.sql.functions import udf

vector_dense_udf = udf(lambda r : Vectors.dense(r),VectorUDT())
data = data.withColumn('hfeatures_dense',vector_dense_udf('hfeatures'))
```

Now we can build the pipeline to scale HLF and encode the labels

In [11]:
```
from pyspark.ml import Pipeline
from pyspark.ml.feature import OneHotEncoderEstimator
from pyspark.ml.feature import MinMaxScaler

## One-Hot-Encode
encoder = OneHotEncoderEstimator(inputCols=["label"],
                                 outputCols=["encoded_label"],
                                 dropLast=False)

## Scale feature vector
scaler = MinMaxScaler(inputCol="hfeatures_dense",
                      outputCol="HLF_input")

pipeline = Pipeline(stages=[encoder, scaler])

%time fitted_pipeline = pipeline.fit(data)
```

```
CPU times: user 294 ms, sys: 293 ms, total: 587 ms
Wall time: 1min 34s
```

In [12]:
```
data = fitted_pipeline.transform(data)
```

Performance - Lessons Learned

- Data preparation is CPU bound
  - Heavy serialization-deserialization due to Python UDF
- Ran using 400 cores: data ingestion took ~3 hours
- It can be optimized, but is it worth it ?
  - Use Spark SQL, or Scala instead of Python UDF
  - Optimization: replaced parts of Python UDF code with Spark SQL and higher order functions: run time, from 3 hours to 2 hours

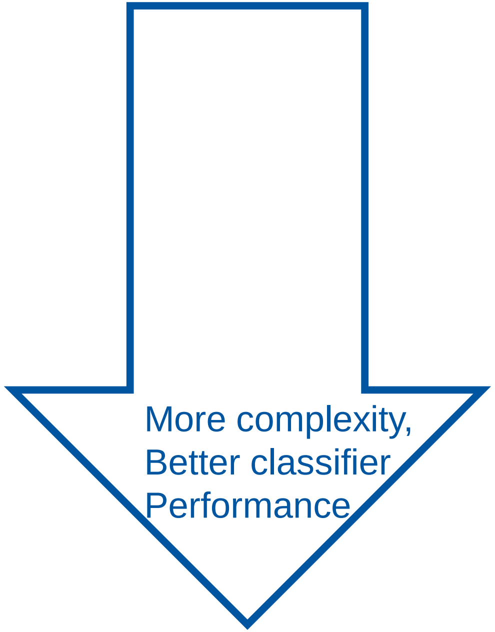
```
FILTER(Electron,
    electron -> electron.PT > 23
) Electron,
FILTER(MuonTight,
    muon -> muon.PT > 23
) MuonTight
```

```
WHERE cardinality(Electron) > 0
      OR cardinality(MuonTight) > 0
```

Development Practices

- Development, start small
  - Use a subset of data for development
  - Use SWAN or a local laptop/desktop
- Run at scale on clusters
  - Same code runs at scale on clusters: YARN, K8S
  - Smooth transition, need for some additional config (e.g. memory)
- API and code lifecycle
  - Spark DataFrame API is stable and popular
  - Improve collaboration with different teams, reproducibility, maintainability

Neural Network Models



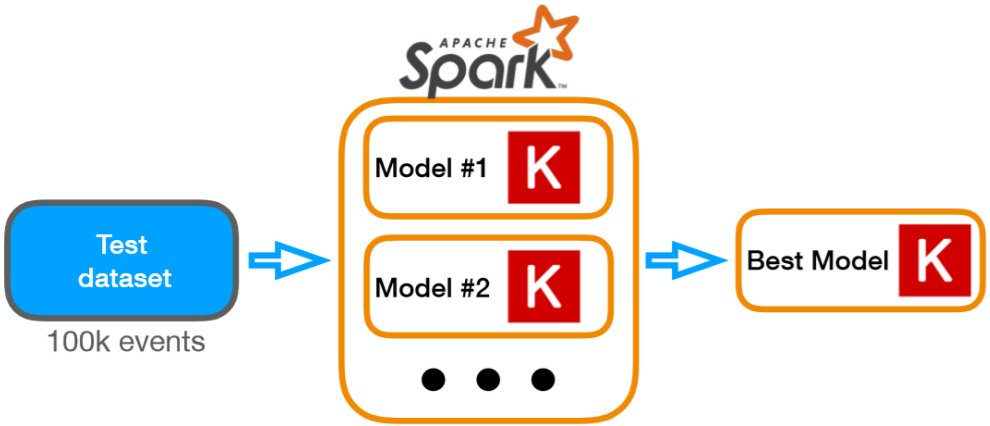
1. Fully connected feed-forward deep neural network
   - Trained using High Level Features (~1 GB of data)

2. Neural network based on Gated Recurrent Unit (GRU)
   - Trained using Low Level Features (~ 300 GB of data)

3. Inclusive classifier model
   - Combination of (1) + (2)

Hyper-Parameter Tuning– DNN

- Hyper-parameter tuning of the DNN model
  - Trained with a subset of the data (cached in memory)
  - Parallelized with Spark, using spark_sklearn.grid_search
    - And scikit-learn + keras: tensorflow.keras.wrappers.scikit_learn



Deep Learning at Scale with Spark

- Investigations and constraints for our exercise
- How to run deep learning in a Spark data pipeline?
  - Neural network models written using Keras API
  - Deploy on Hadoop and/or Kubernetes clusters (CPU clusters)
- Distributed deep learning
  - GRU-based model is complex
  - Slow to train on a single commodity (CPU) server

Spark, Analytics Zoo and BigDL

- Apache Spark
  - Leading tool and API for data processing at scale
- Analytics Zoo is a platform for **unified** analytics and AI
  - Runs on Apache Spark leveraging BigDL / Tensorflow
  - For service developers: integration with infrastructure (hardware, data access, operations)
  - For users: Keras APIs to run user models, integration with Spark data structures and pipelines
- BigDL is an open source distributed deep learning framework for Apache Spark

BigDL Runs as Standard Spark Programs

Standard Spark jobs

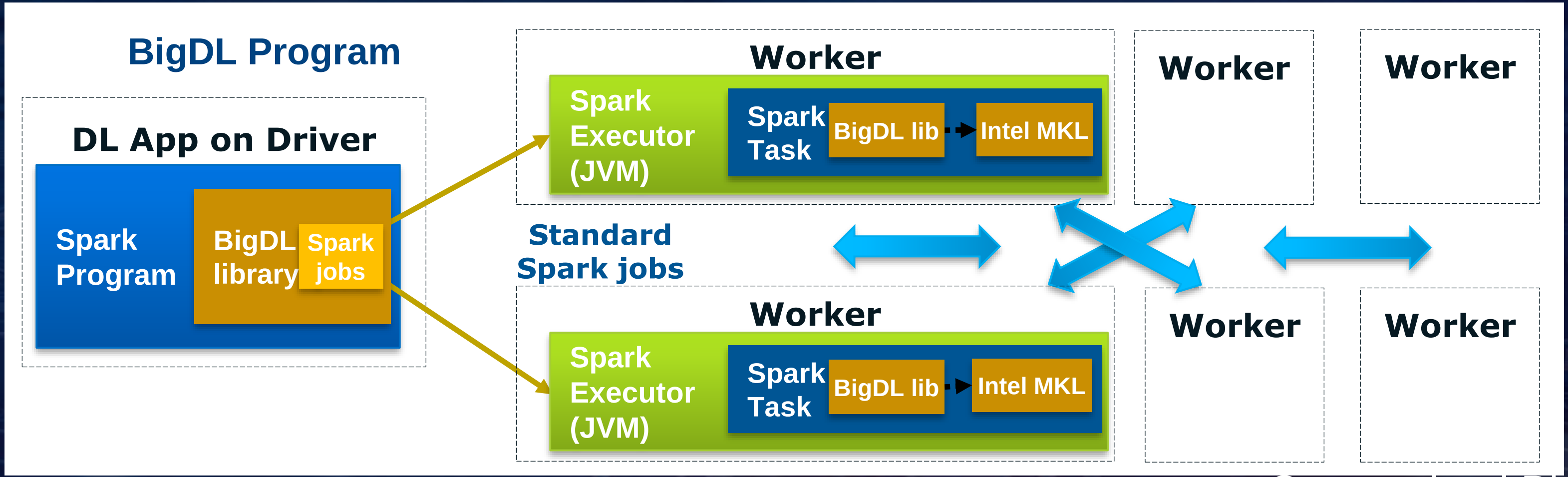
- No changes to the Spark or Hadoop clusters needed

Iterative

- Each iteration of the training runs as a Spark job

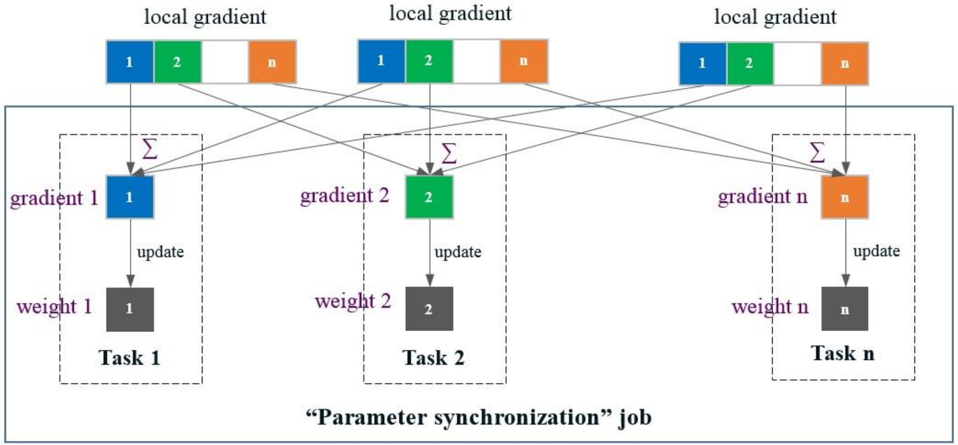
Data parallel

- Each Spark task runs the same model on a subset of the data (batch)



Source: Intel BigDL Team

BigDL Parameter Synchronization




```
For each task n in the "parameter synchronization" job
    shuffle the n^th partition of all gradients to this task
    aggregate (sum) the gradients
    updates the n^th partition of the weights
    broadcast the n^th partition of the updated weights
}
```

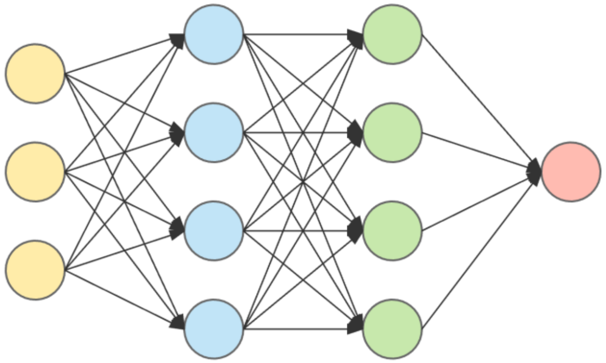
Source: https://github.com/intel-analytics/BigDL/blob/master/docs/docs/whitepaper.md

Model Development – DNN for HLF

- Model is instantiated using the Keras-compatible API provided by Analytics Zoo

In [7]:
```
# Create keras like zoo model.
# Only need to change package name from keras to zoo.pipeline.api.keras

from zoo.pipeline.api.keras.optimizers import Adam
from zoo.pipeline.api.keras.models import Sequential
from zoo.pipeline.api.keras.layers.core import Dense, Activation

model = Sequential()
model.add(Dense(50, input_shape=(14,), activation='relu'))
model.add(Dense(20, activation='relu'))
model.add(Dense(10, activation='relu'))
model.add(Dense(3, activation='softmax'))
```

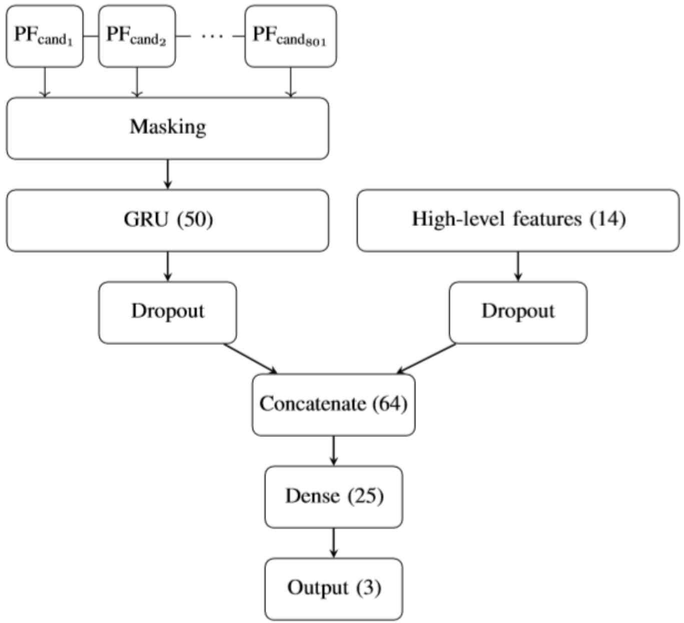
```
creating: createZooKerasSequential
creating: createZooKerasDense
creating: createZooKerasDense
creating: createZooKerasDense
creating: createZooKerasDense
```



Model Development – GRU + HLF

A more complex network topology, combining a GRU of Low Level Feature + a DNN of High Level Features

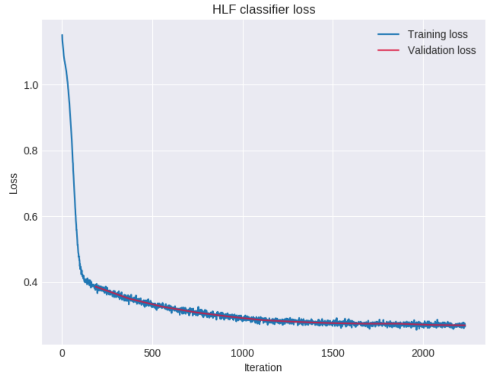
```
from zoo.pipeline.api.keras.optimizers import Adam
from zoo.pipeline.api.keras.models import Sequential
from zoo.pipeline.api.keras.layers.core import *
from zoo.pipeline.api.keras.layers.recurrent import GRU
from zoo.pipeline.api.keras.engine.topology import Merge

## GRU branch
gruBranch = Sequential() \
            .add(Masking(0.0, input_shape=(801, 19))) \
            .add(GRU(
                output_dim=50,
                activation='tanh'
            )) \
            .add(Dropout(0.2)) \

## HLF branch
hlfBranch = Sequential() \
            .add(Dropout(0.2, input_shape=(14,)))

## Concatenate the branches
branches = Merge(layers=[gruBranch, hlfBranch], mode='concat')

## Create the model
model = Sequential() \
        .add(branches) \
        .add(Dense(25, activation='relu')) \
        .add(Dense(3, activation='softmax'))
```



Distributed Training

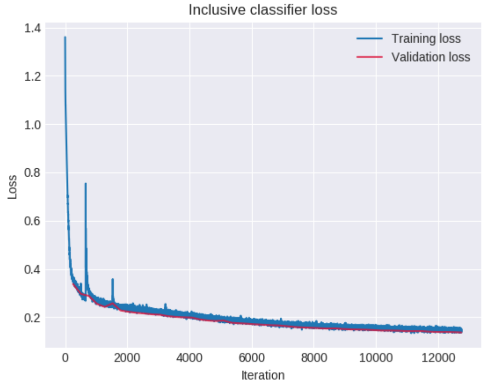
Instantiate the estimator using Analytics Zoo / BigDL

```
# Create SparkML compatible estimator for deep learning training

from bigdl.optim.optimizer import EveryEpoch, Loss, TrainSummary, ValidationSummary
from zoo.pipeline.nnframes import *
from zoo.pipeline.api.keras.objectives import CategoricalCrossEntropy

estimator = NNEstimator(model, CategoricalCrossEntropy())\
        .setOptimMethod(Adam()) \
        .setBatchSize(BDLbatch) \
        .setMaxEpoch(numEpochs) \
        .setFeaturesCol("HLF_input") \
        .setLabelCol("encoded_label") \
        .setValidation(trigger=EveryEpoch() , val_df=testDF,
                       val_method=[Loss(CategoricalCrossEntropy())], batch_size=BDLbatch)
```



The actual training is distributed to Spark executors

```
%%time
trained_model = estimator.fit(trainDF)
```



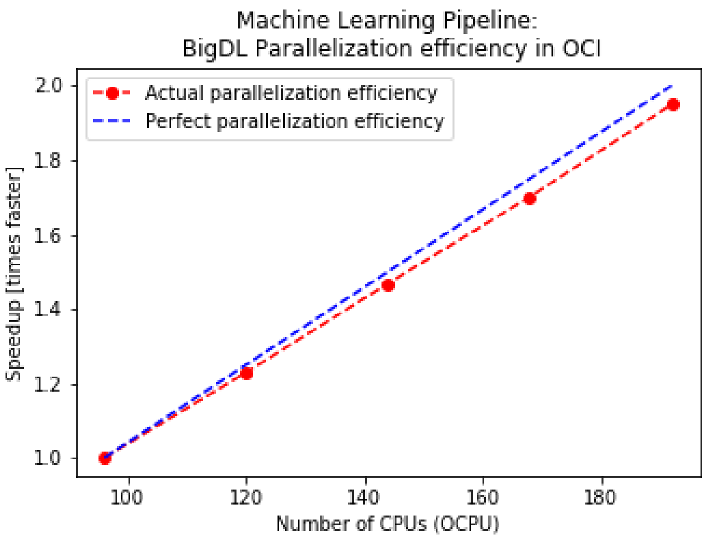
Storing the model for later use

```
modelDir = logDir + '/nnmodels/HLFClassifier'
trained_model.save(modelDir)
```

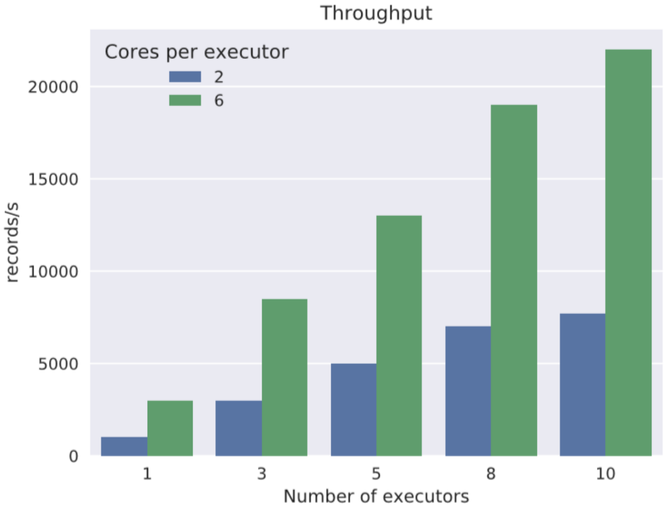
Performance and Scalability of Analytics Zoo/BigDL

Analytics Zoo/BigDL on Spark scales up in the ranges tested

Inclusive classifier model

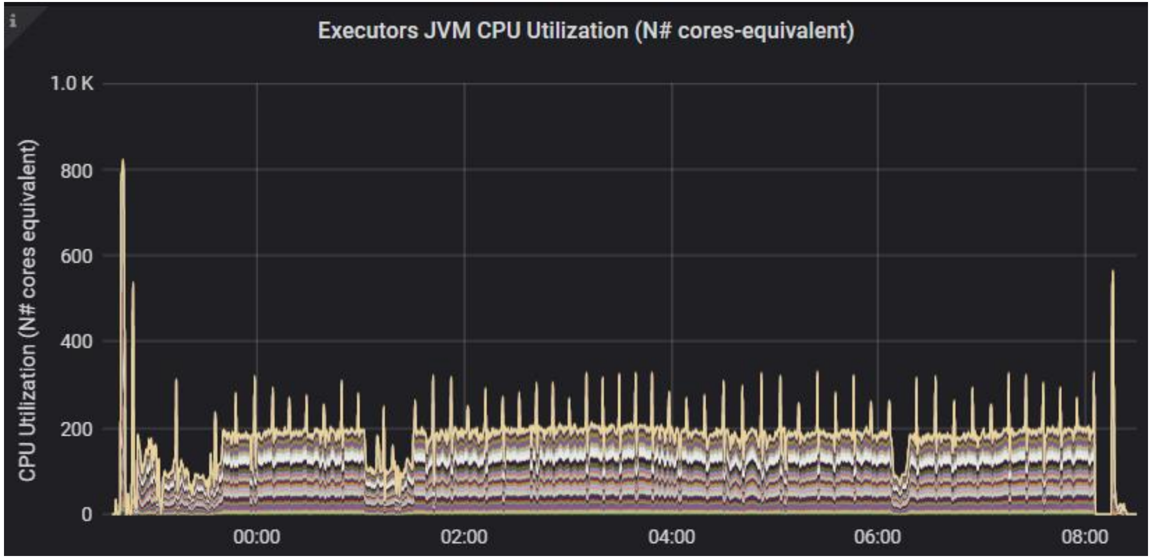


DNN model, HLF features



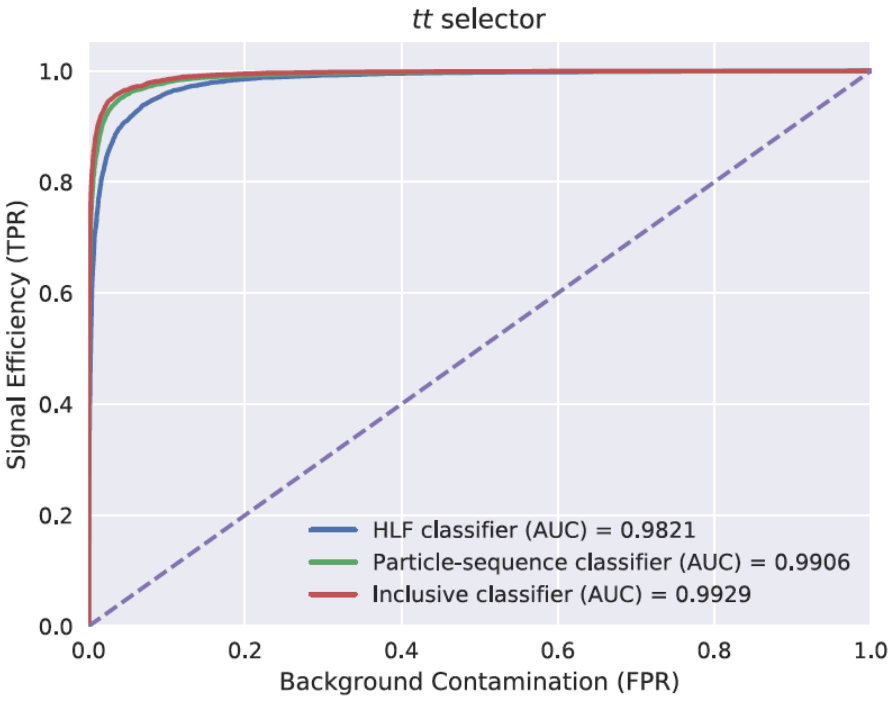
Workload Characterization

- Training with Analytics zoo
  - GRU-based model: Distributed training on YARN cluster
  - Measure with Spark Dashboard: it is CPU bound



Results – Model Performance

- Trained models with Analytics Zoo and BigDL
- Met the expected results for model performance: ROC curve and AUC



Spark + TensorFlow

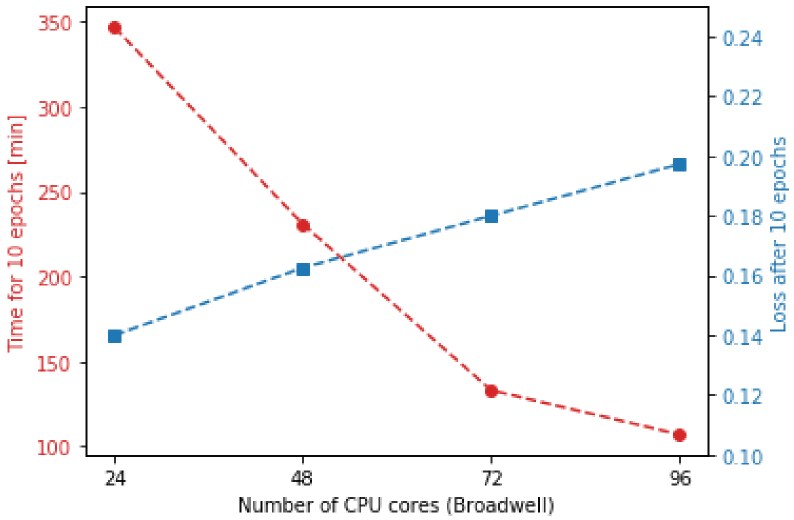
- Additional tests on different architecture
  - Data preparation ->
  - Exchange data with TFRecord format
  - Distributed DL ->

Training with TensorFlow 2.0

- Training and test data
  - Converted from Parquet to TFRecord format using Spark
  - TensorFlow: data ingestion using tf.data and tf.io
- Distributed training with tf.distribute + tool for K8S: https://github.com/cerndb/tf-spawner

Distributed training with TensorFlow 2.0 on Kubernetes (CERN cloud)

TF 2.0 feature:
`tf.distribute.experimental.MultiWorkerMirroredStrategy`



Performance and Lessons Learned

- Measured distributed training elapsed time
  - From a few hours to 11 hours, depending on model, number of epochs and batch size. Hard to compare different methods and solutions (many parameters)

- Distributed training with BigDL and Analytics Zoo
  - Integrates very well with Spark
  - Need to cache data in memory
  - Noisy clusters with stragglers can add latency to parameter synchronization

- TensorFlow 2.0
  - It is straightforward to distribute training on CPUs and GPUs with tf.distribute
  - Data flow: Use TFRecord format, read with TensorFlow's tf.data and tf.io
  - GRU training performance on GPU: 10x speedup in TF 2.0
    - Training of the Inclusive Classifier on a single P100 in 5 hours

Recap: our Deep Learning Pipeline

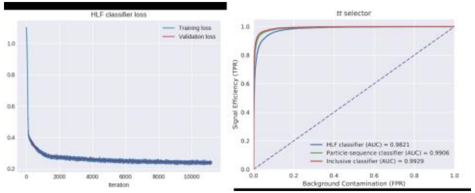
Data and models from Research

Input: labeled data and DL models

Feature engineering at scale

Hyperparameter optimization (Random/Grid search)

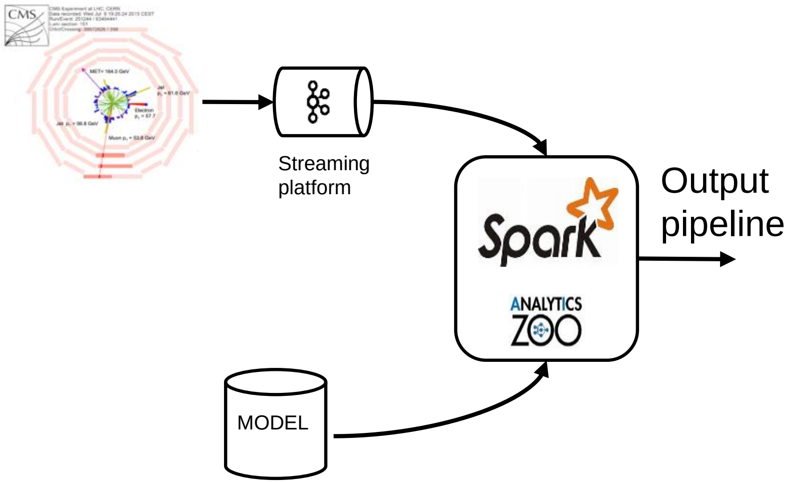
Distributed model training



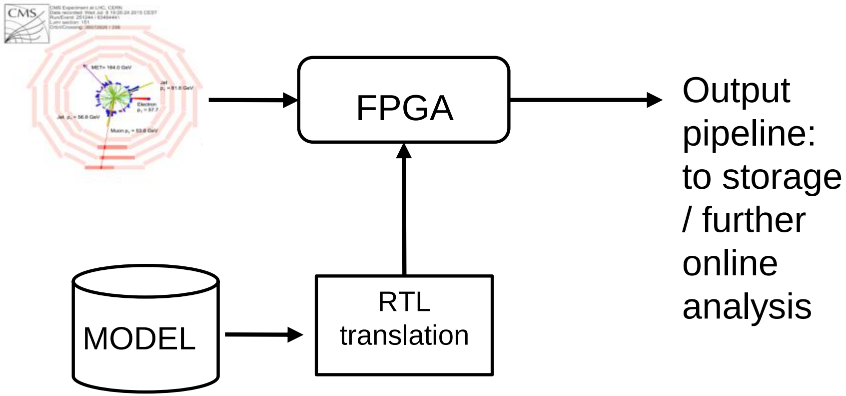
Output: particle selector model

Model Serving and Future Work

- Using Apache Kafka and Spark?



- FPGA serving DNN models



End-To-End ML Pipeline Summary

- Spark, Python notebooks
  - Provide well-known APIs and productive environment for data preparation
- Data preparation performance, lessons learned:
  - Use Spark SQL/DataFrame API, avoid Python UDF when possible
- Successfully scaled Deep Learning on Spark clusters
  - Using Analytics Zoo and BigDL
  - Deployed on existing Intel Xeon-based servers: Hadoop clusters and cloud
- Good results also with Tensorflow 2.0, running on Kubernetes
  - GPU resources are important for DL
- We have only explored some of the available solutions
  - Data preparation and scalable + distributed training are key

Services and Resources

Users of Big Data Platforms

- Many use cases at CERN for analytics
  - Data analysis, dashboards, plots, joining and aggregating multiple data, libraries for specialized processing, machine learning, …
- Communities
  - Physics:
    - Analytics on computing data (e.g. studies of popularity, grid jobs, file transfers, etc) (CMS Spark project, ATLAS Rucio)
    - Parallel processing of ROOT RDataframes with PyRDF for data analysis
    - Development of new ways to process Physics data, e.g.: data reduction and analysis with spark-ROOT, more recently Coffea and Laurelin by LHC Bigdata project
    - ATLAS EventIndex project
  - IT:
    - Analytics on IT monitoring data
    - Computer security
  - BE:
    - NXCALS – next generation accelerator logging platform
    - BE controls data and analytics

Hadoop and Spark Service at CERN IT

- Setup and run the infrastructure
- Support user community
  - Provide consultancy
  - Doc and training

- Facilitate use
  - Package libraries and configuration
  - Client machines + Docker clients
  - Notebook service integration
  - https://hadoop.web.cern.ch
  - https://hadoop-user-guide.web.cern.ch

Hadoop service in numbers

6 clusters
- 4 production (bare-metal)
- 2 QA clusters (VMs)

140+ physical servers

40+ virtual machines

28+ PBs of Storage

40+ TB of Memory

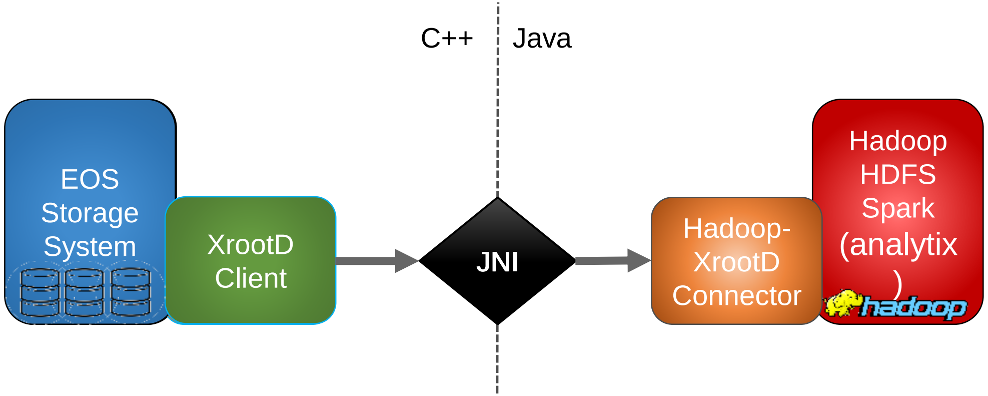
4000+ physical cores

HDDs and SSDs

Data growth: ~8 TB per day

XRootD connector for Hadoop and Spark

- A library that binds Hadoop-based file system API with XRootD native client
  - Developed by CERN IT
- Allows most of components from Hadoop stack (Spark, MapReduce, Hive etc) to read/write from EOS and CASTOR directly
  - No need to copy the data to HDFS before processing
  - Works with Grid certificates and Kerberos for authentication



Spark as a service on a private cloud

- Under R&D since 2018, rolled out in 2019
- Appears to be a good solution when data locality is not needed
  - CPU and memory intensive rather than IO intensive workloads
  - Reading from storage systems via network (EOS, S3, “foreign” HDFS)
  - Compute resources can be flexibly scaled out

- Spark clusters – on cloud containers
  - Kubernetes on Openstack
  - Spark runs on Kubernetes since version 2.3
- Use cases
  - SWAN integration for users reading from EOS
  - High demand of computing resources, needing to used cloud resources
  - Streaming jobs (e.g. accessing Apache Kafka)

Spark Clusters at CERN: on Hadoop and on Cloud

- Clusters run on
  - Hadoop clusters: Spark on YARN
  - Cloud: Spark on Kubernetes
- Hardware: commodity servers, continuous refresh and capacity expansion

NXCals for Accelerator Logging (part of LHC infrastructure)	Hadoop - YARN – 32 nodes (Cores - 1024, Mem - 16 TB, Storage – 7.5 PB)
General Purpose	Hadoop - YARN, 54 nodes (Cores – 1184, Mem – 21 TB, Storage – 11 PB)
Cloud containers	Kubernetes on Openstack VMs, Cores - 250, Mem – 2 TB Storage: remote HDFS or EOS (for physics data)

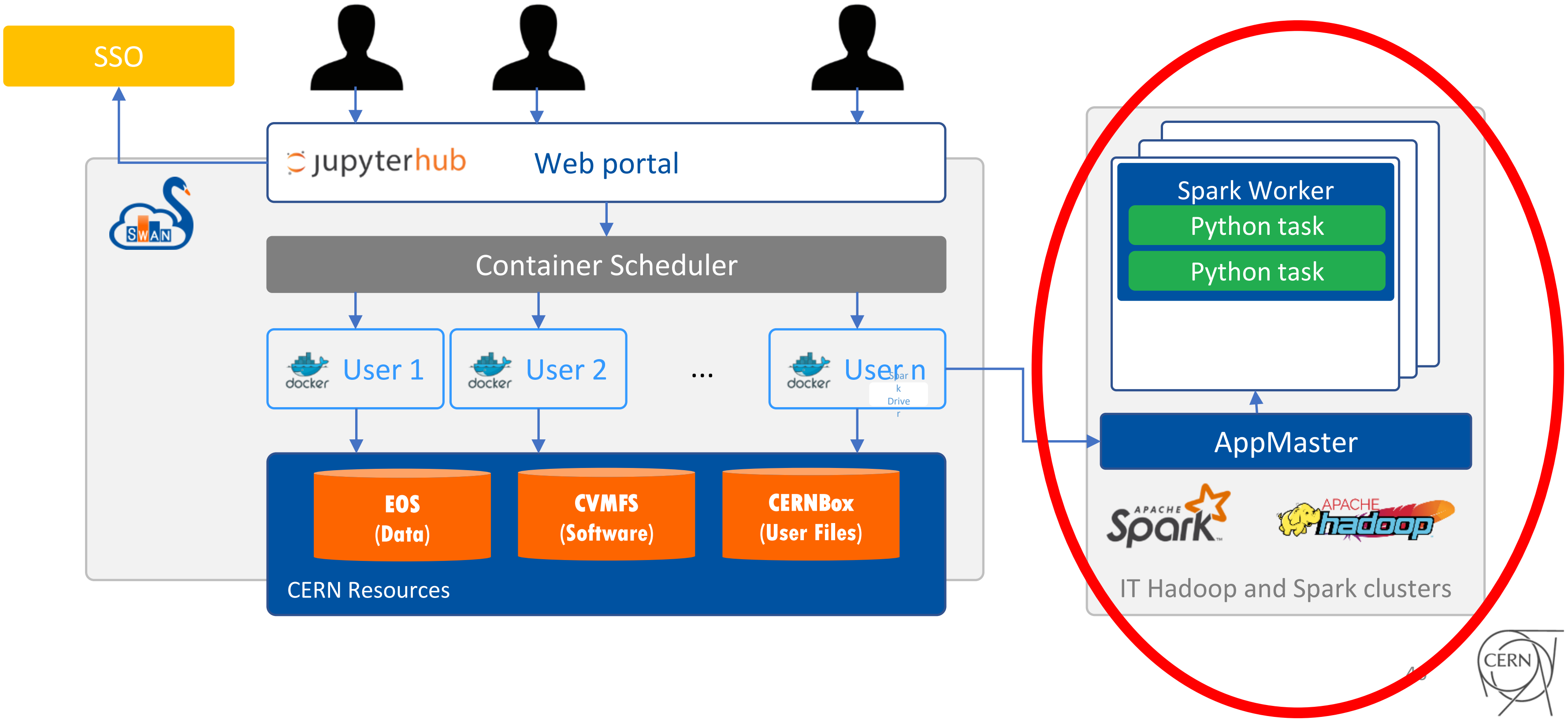
SWAN – Jupyter Notebooks On Demand

- Service for web based analysis (SWAN)
  - Developed at CERN, initially for physics analysis by EP-SFT

- An interactive platform that combines code, equations, text and visualizations
  - Ideal for exploration, reproducibility, collaboration

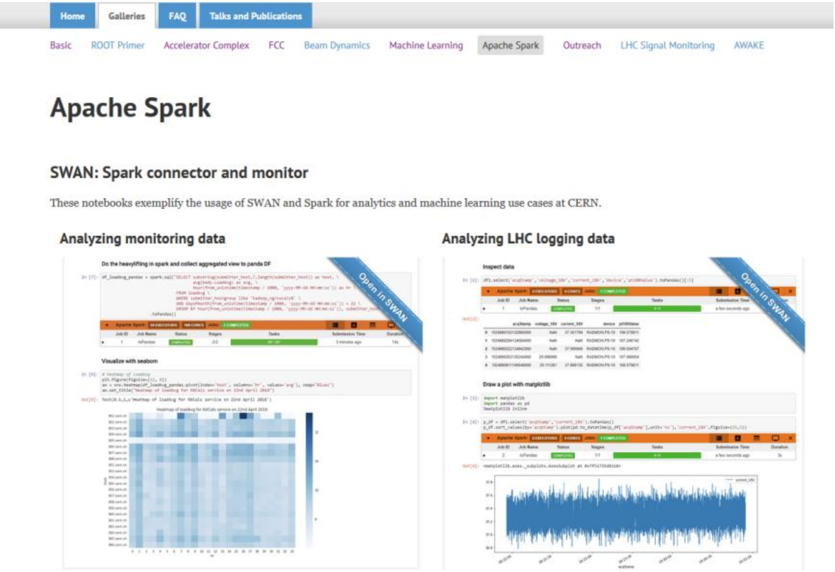
- Fully integrated with Spark and Hadoop service
  - Python on Spark (PySpark) at scale
  - Modern, powerful and scalable platform for data analysis
  - Web-based: no need to install any software

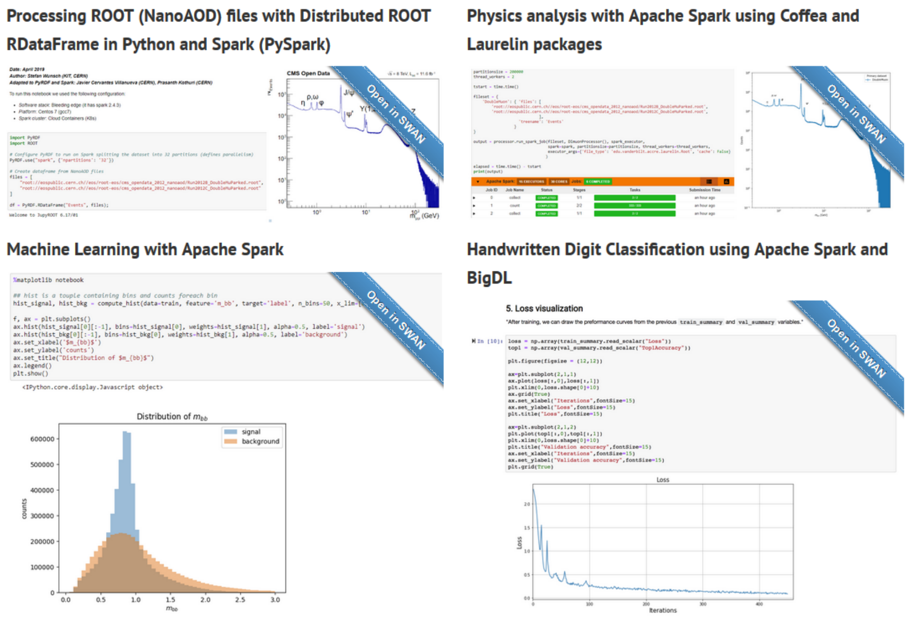
Spark Integration in the SWAN Architecture



Example Notebooks

https://swan.web.cern.ch/content/apache-spark





Why Spark?

- Data processing at scale
  - DataFrames, similar to Pandas
  - You cannot “fit the problem on a laptop”
- Machine Learning at scale
  - “scikit-learn” at scale
- Data Streaming
- One tool with many features
  - Popular API

Image Credit: Vector Pocket Knife from Clipart.me

What Can be Improved?

- Spark runs natively on JVM
  - Python integration is key at CERN. Works OK but performance still needs to improve
- Spark is most useful at scale
  - We see many ML tasks that fit in a server
- Spark and GPUs
  - Work in progress. Horovod on Spark is a possibility
- Competition
  - Cloud and open source tools: Kubeflow, DASK, …

Areas for Future Development

- Further improve the analytics platform
  - Use of cloud resources, also testing public clouds
  - Integration of GPUs
- Machine Learning
  - Collect feedback from users communities
  - Are tools at scale useful?
  - What are the main use cases?
  - What is missing in the platform?

Conclusions

- End-to-end pipeline for machine learning
  - Developed with Apache Spark, BigDL and Tensorflow, using Jupyter/Python,
- Big Data tools and platforms at CERN
  - For data analysis, machine learning and streaming
  - Run at scale on YARN and on Kubernetes
  - Integrate with CERN computing environment

Acknowledgments and Links

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- Authors of “Topology classification with deep learning to improve real-time event selection at the LHC”, notably Thong Nguyen, Maurizio Pierini
- Intel team for BigDL and Analytics Zoo: Jiao (Jennie) Wang, Sajan Govindan

ML Pipeline:

- Data and code: https://github.com/cerndb/SparkDLTrigger
- Machine Learning Pipelines with Modern Big Data Tools for High Energy Physics http://arxiv.org/abs/1909.10389

CERN Spark and Hadoop Service:

- https://hadoop-user-guide.web.cern.ch/hadoop-user-guide/getstart/access.html
- Spark on SWAN: https://swan.web.cern.ch/content/apache-spark