SPARK+AI
SUMMIT 2019

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Deep Learning Pipelines for High Energy Physics using Apache Spark with Distributed Keras and Analytics Zoo

Luca Canali, CERN

#UnifiedDataAnalytics #SparkAISummit

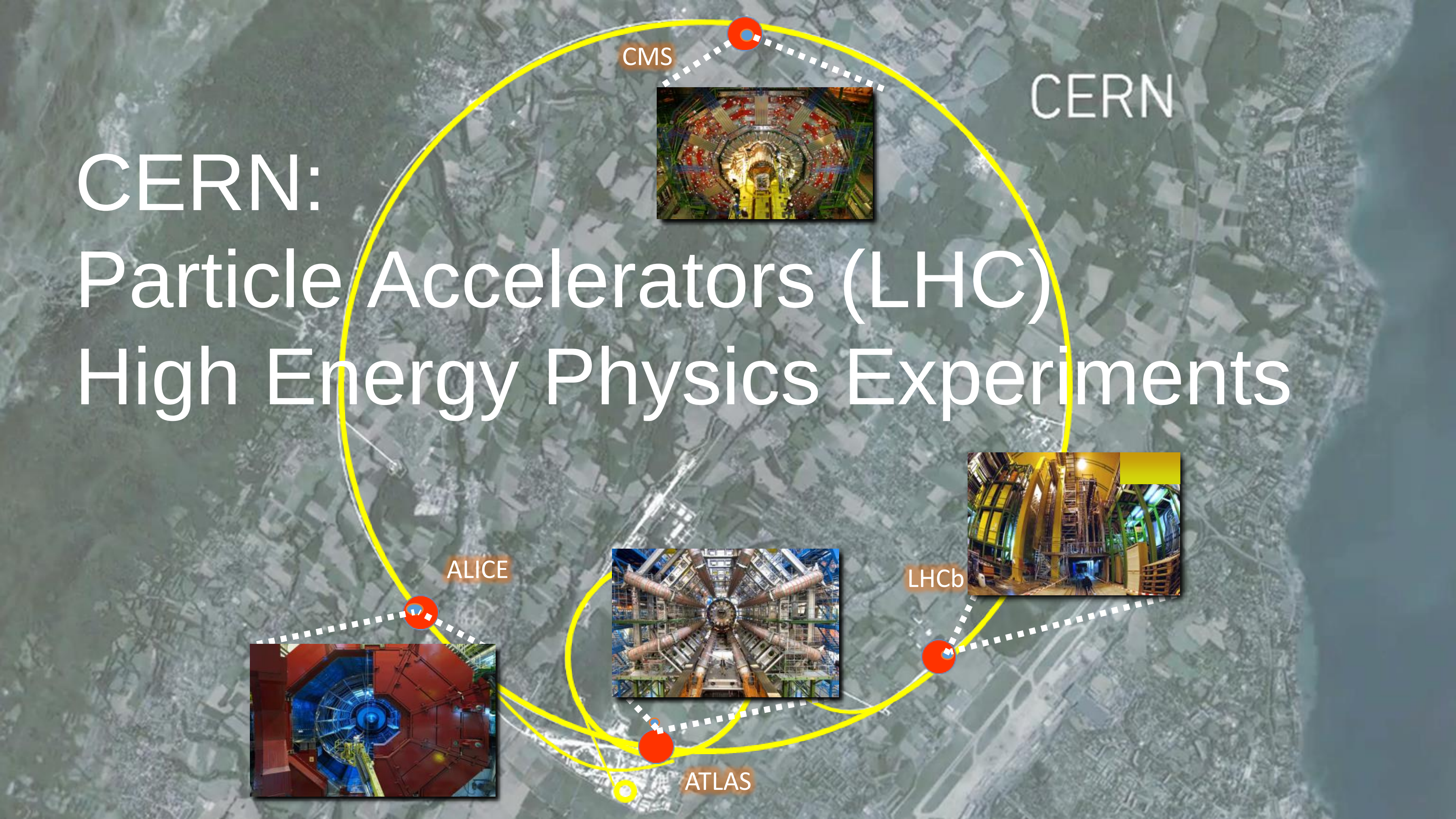
SPARK+AI SUMMIT 2019

About Luca

- Data Engineer at CERN
  - Hadoop and Spark service, database services
  - 19+ years of experience with data engineering
- Sharing and community
  - Blog, notes, tools, contributions to Apache Spark

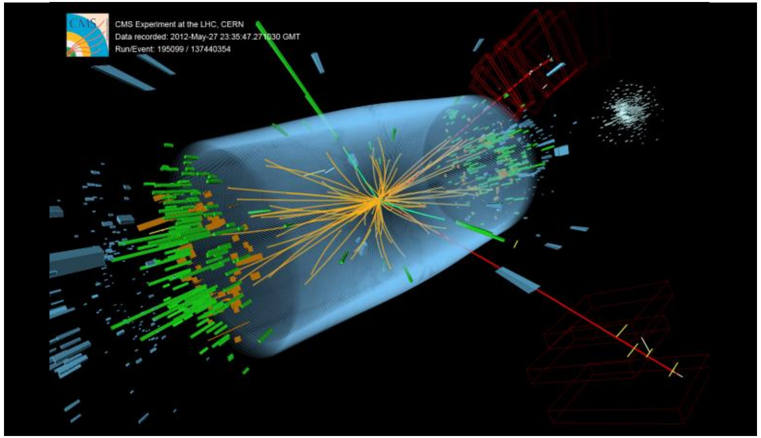
@LucaCanaliDB – http://cern.ch/canali

CERN:
Particle Accelerators (LHC)
High Energy Physics Experiments



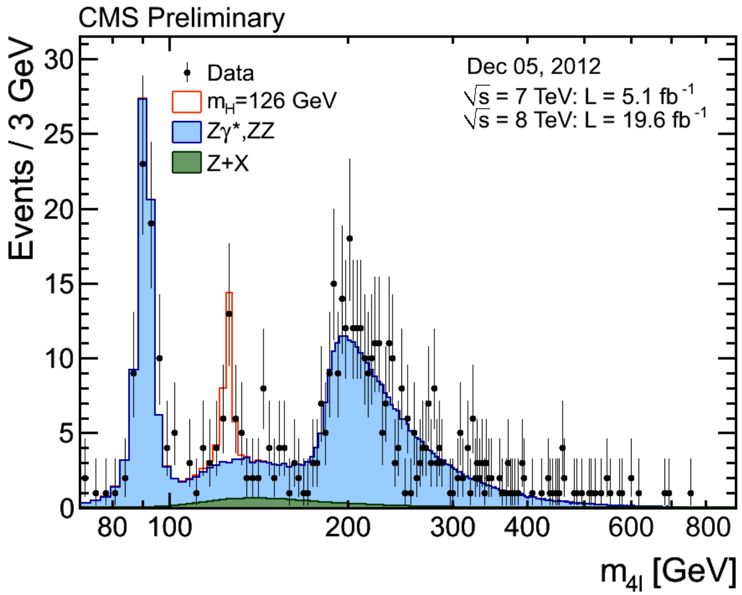
Experimental High Energy Physics is Data Intensive

Particle Collisions



Large Scale Computing

Physics Discoveries

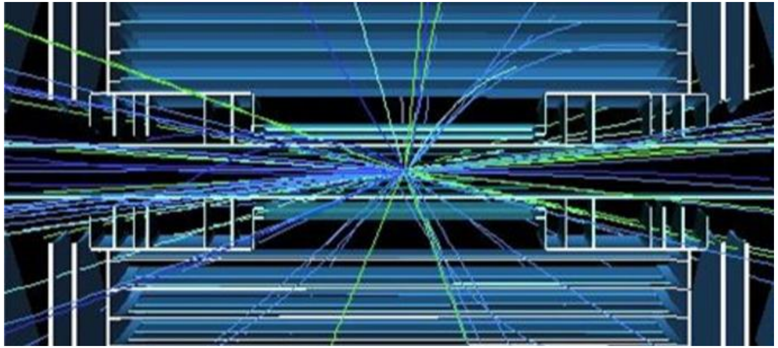


https://twiki.cern.ch/twiki/pub/CMSPublic/Hig13002TWiki/HZZ4l_animated.gif

And https://iopscience.iop.org/article/10.1088/1742-6596/455/1/012027

Key Data Processing Challenge

- Proton-proton collisions at LHC experiments happen at 40MHz.
  - Hundreds of TB/s of electrical signals that allow physicists to investigate particle collision events.
- Storage, limited by bandwidth
  - Currently, only 1 every ~40K events stored to disk (~10 GB/s).



2018: 5 collisions/beam cross
Current LHC

2026: 400 collisions/beam cross
Future: High-Luminosity LHC upgrade

CERN

Data Flow at LHC Experiments

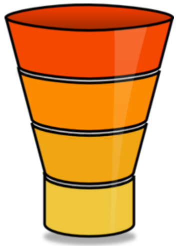
40 million collisions per second (Raw) → PB/s → 100,000 selections per second (L1) → TB/s → 1,000 selections per second (L2) → GB/s

This can generate up to a petabyte of raw data per second

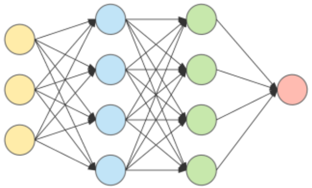
Reduced to GB/s by filtering in real time

Key is how to select potentially interesting events (trigger systems).

R&D – Data Pipelines



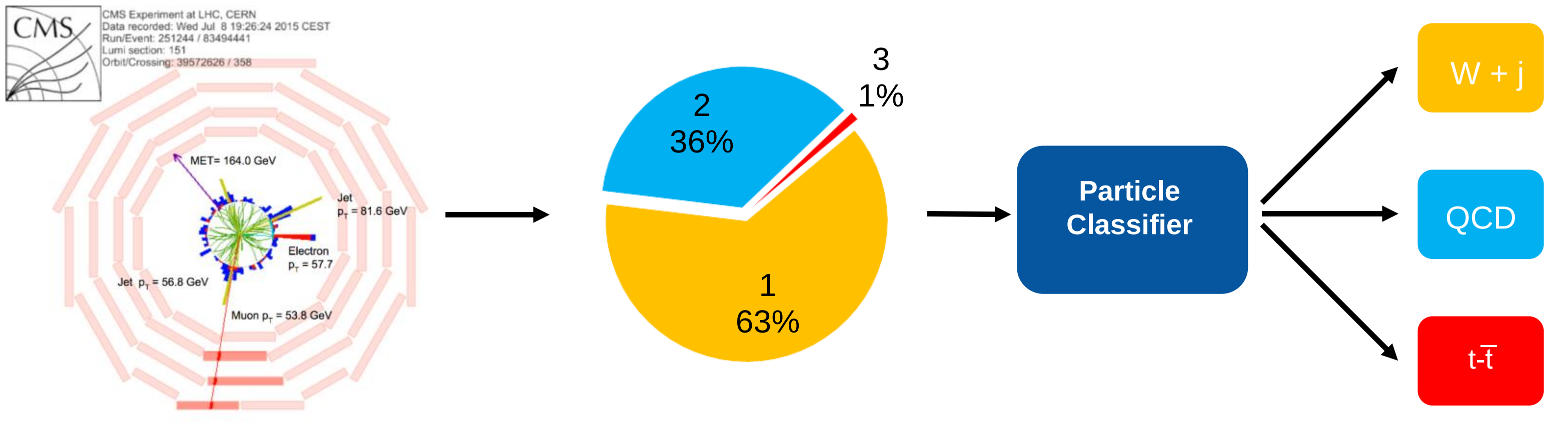
- Improve the **quality of filtering systems**
  - Reduce false positive rate
  - From rule-based algorithms to classifiers based on Deep Learning



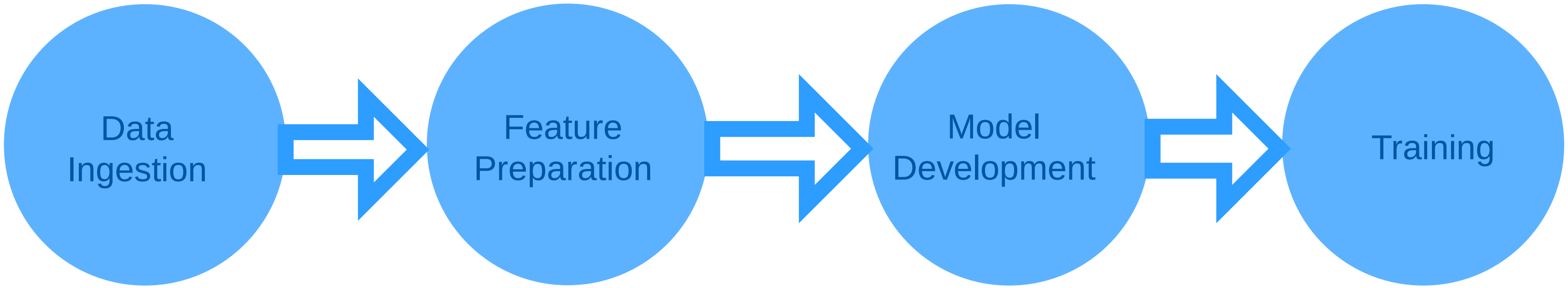
- Advanced analytics **at the edge**
  - Avoid wasting resources in offline computing
  - Reduction of operational costs

Particle Classifiers 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**



Deep Learning Pipeline for Physics Data



Data Ingestion: Read physics data and feature engineering

Feature Preparation: Prepare input for Deep Learning network

Model Development:
1. Specify model topology
2. Tune model topology on small dataset

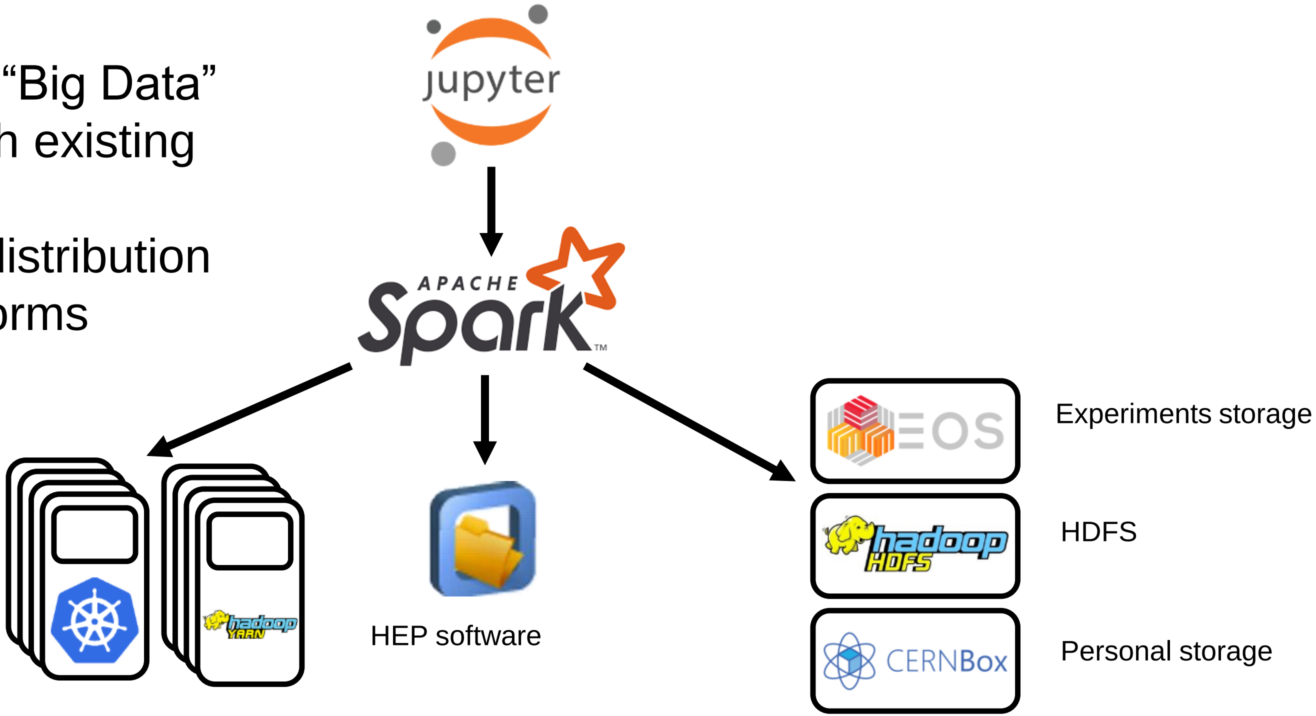
Training: Train the best model

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

Analytics Platform at CERN

Integrating new “Big Data” components with existing infrastructure:

- Software distribution
- Data platforms



FILE EDIT VIEW INSERT CELL KERNEL HELP

Trusted | Python 2

Code

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()
```

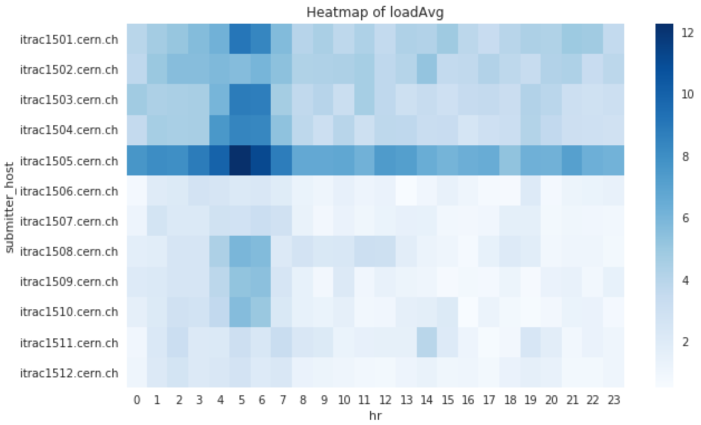
Apache Spark: 90 EXECUTORS 180 CORES Jobs: 1 COMPLETED

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

Hadoop and Spark Clusters at CERN

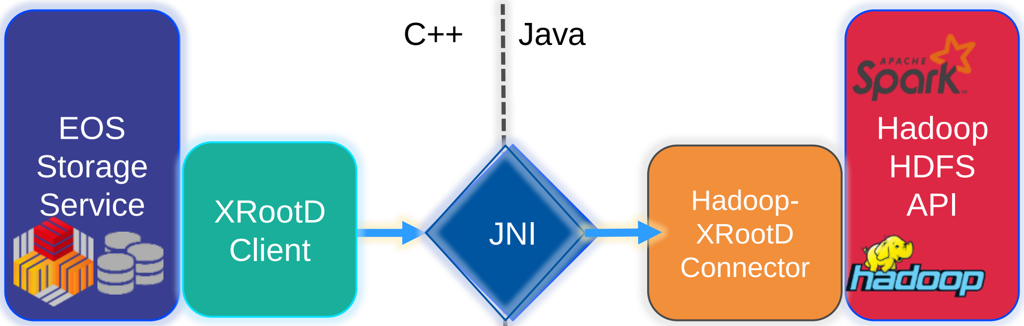
- Clusters:
  - YARN/Hadoop
  - Spark on Kubernetes
- Hardware: Intel based servers, continuous refresh and capacity expansion

Accelerator logging (part of LHC infrastructure)	Hadoop - YARN - 30 nodes (Cores - 1200, Mem - 13 TB, Storage – 7.5 PB)
General Purpose	Hadoop - YARN, 65 nodes (Cores – 2.2k, Mem – 20 TB, Storage – 12.5 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

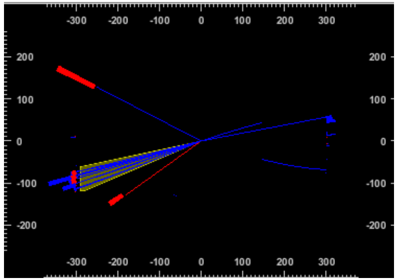
https://github.com/cerndb/hadoop-xrootd
https://github.com/diana-hep/spark-root

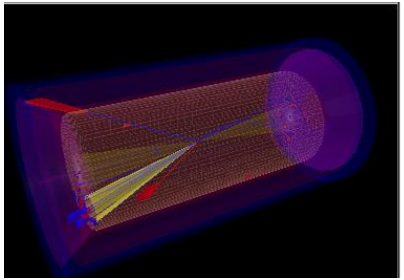


Labeled Data for Training and Test

- 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

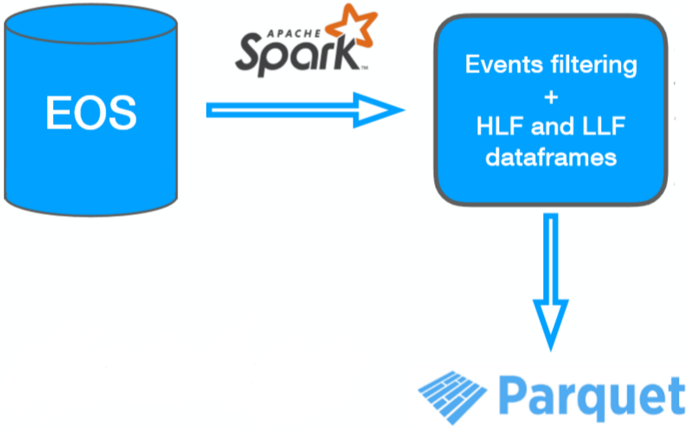




Step 1: Data Ingestion

- Read input files: 4.5 TB from custom (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)

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

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 and 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, Scala instead of Python UDF
  - Optimization: replacing 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
```

Neural Network Models and

Complexity +
Classifier
Performance

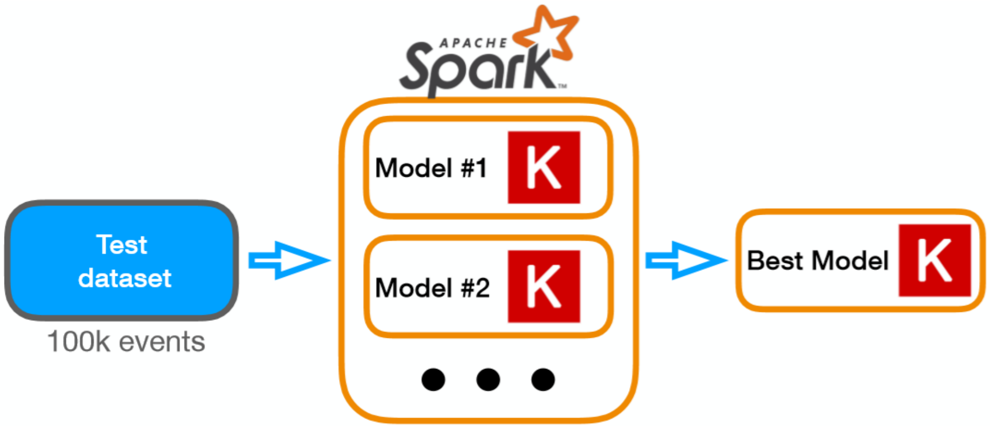
1. Fully connected feed-forward deep neural network
   - Trained using High Level Features (~1 GB of data)

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 Run as Standard Spark Programs

Standard Spark jobs

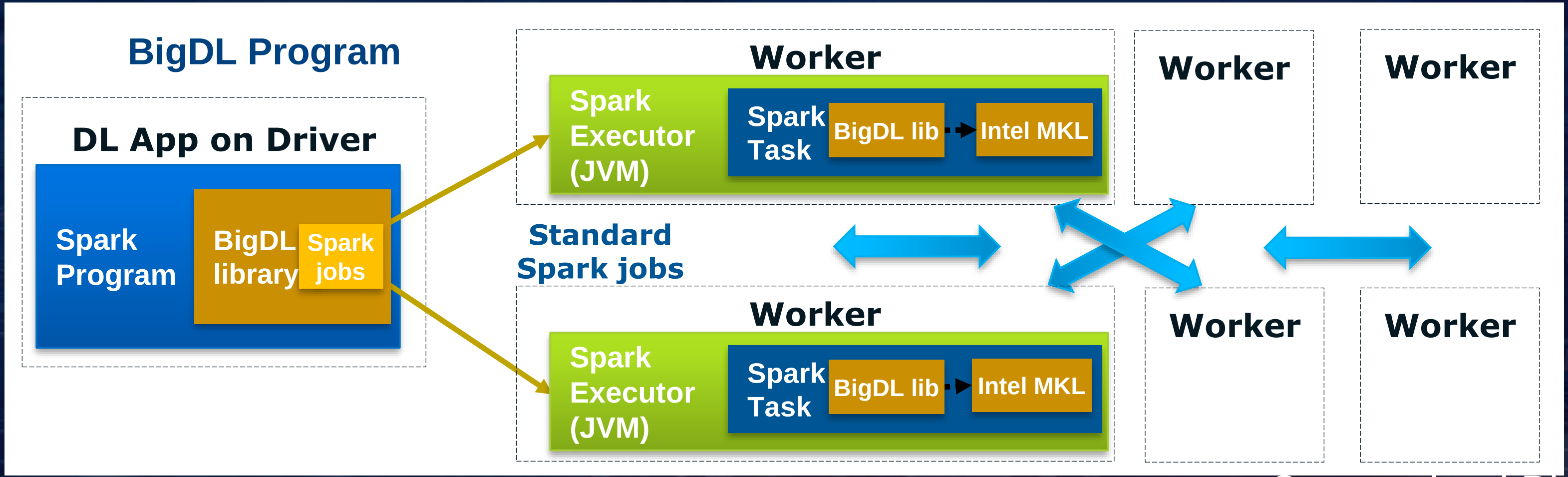
- No changes to the Spark or Hadoop clusters needed

Iterative

- Each iteration of the training runs as a Spark job

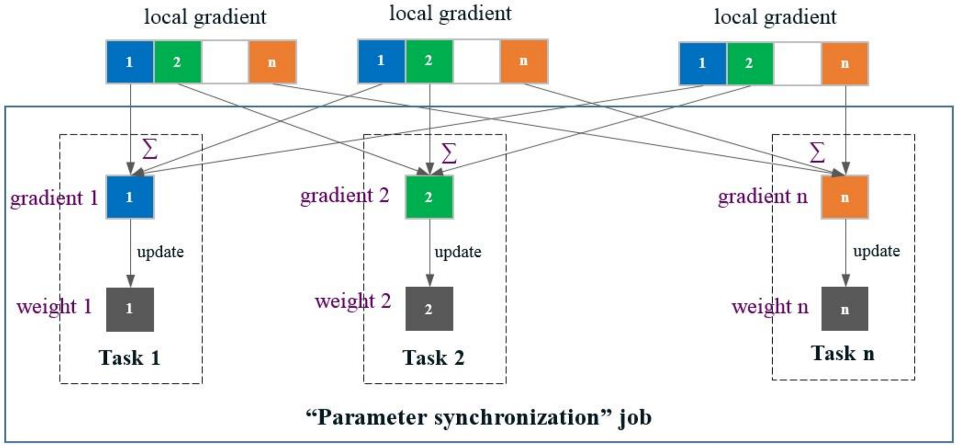
Data parallel

- 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

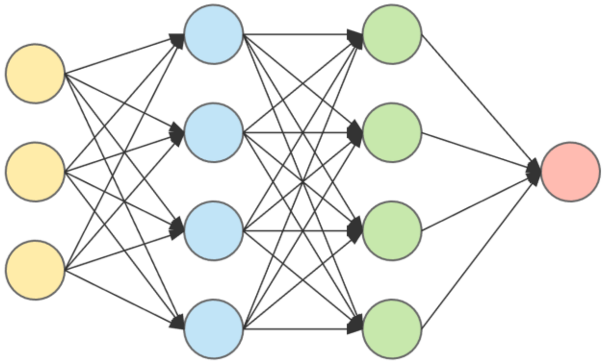
}

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

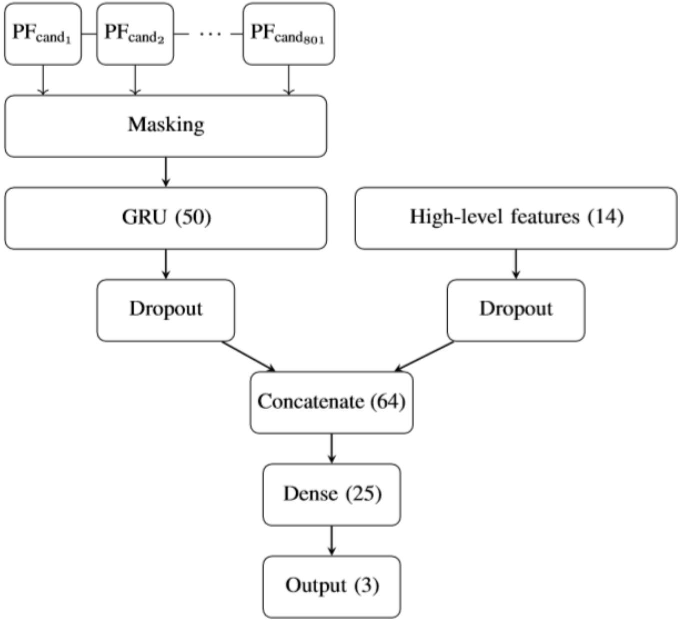
```
In [7]: # Create keras like zoo model.
        # Only need to change package name from keras to zoo.pipeline.api.keras

        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

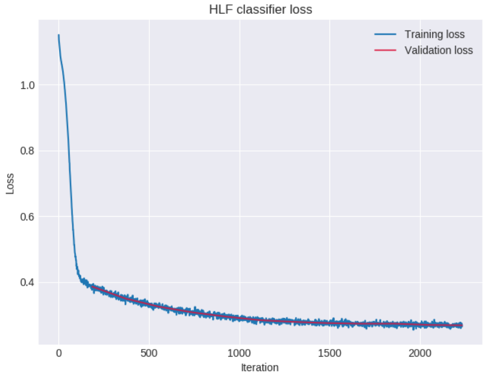
```python
from zoo.pipeline.api.keras.optimizers import Adam
from zoo.pipeline.api.keras.models import Sequential
from zoo.pipeline.api.keras.layers.core import *
from zoo.pipeline.api.keras.layers.recurrent import GRU
from zoo.pipeline.api.keras.engine.topology import Merge

## 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

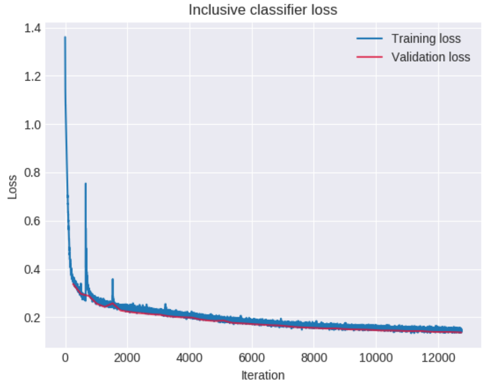
Instantiate the estimator using Analytics Zoo / BigDL

```
# 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)
```



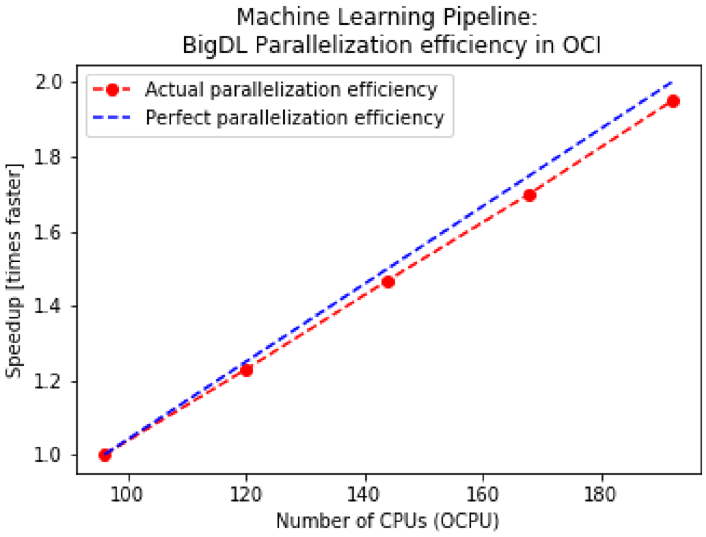
Storing the model for later use

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

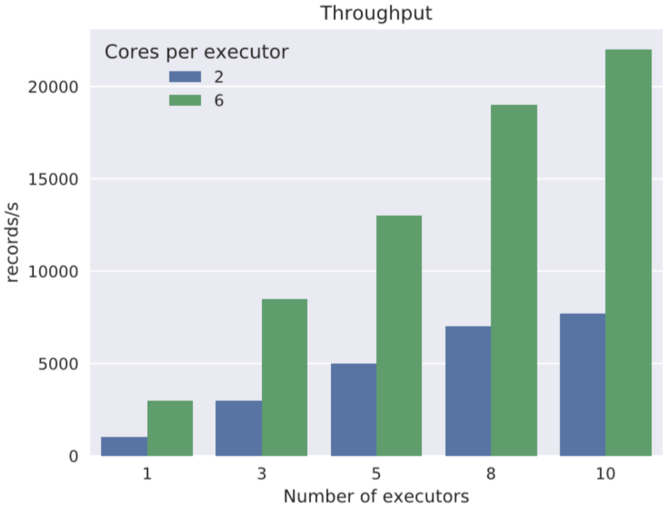
Performance and Scalability of Analytics Zoo/BigDL

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

Inclusive classifier model

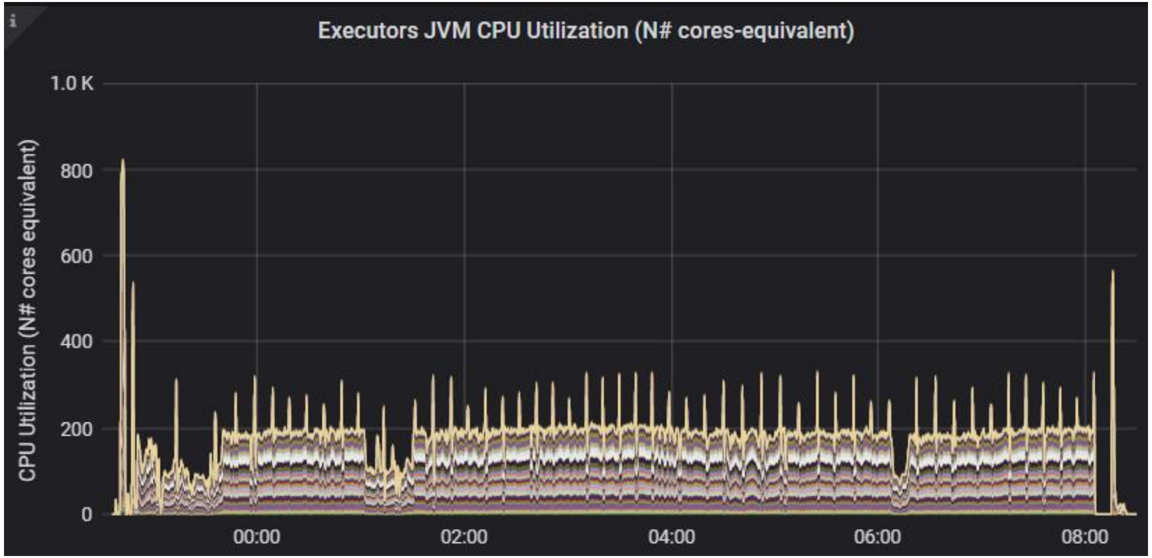


DNN model, HLF features



Workload Characterization

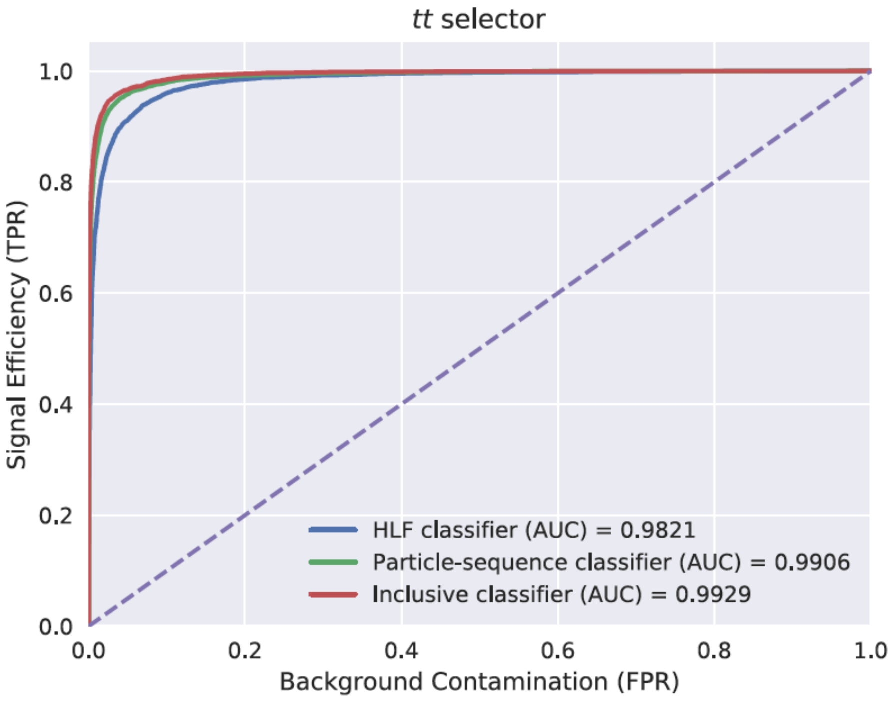
- Training with Analytics zoo
  - GRU-based model: Distributed training on YARN cluster
  - Measure with Spark Dashboard: it is CPU bound



Results – Model Performance

- Trained models with Analytics Zoo and BigDL

- Met the expected results for model performance: ROC curve and AUC

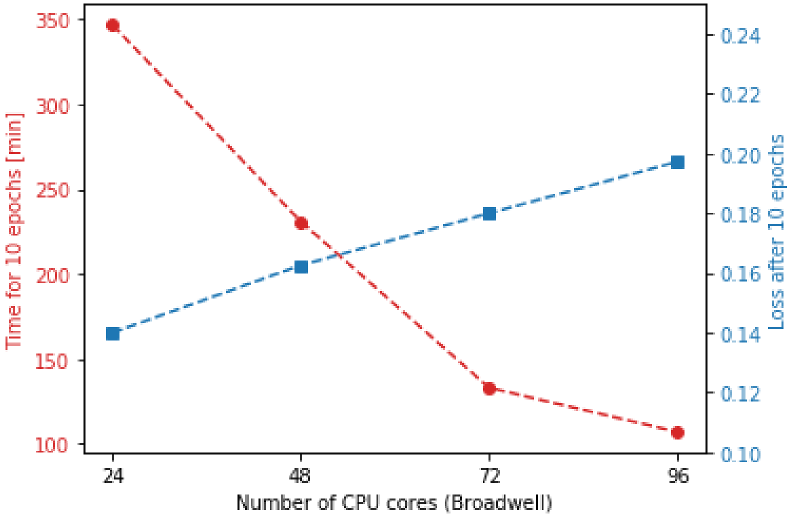


Training with TensorFlow 2.0

- 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)

Distributed training of the Keras model with:
`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 with Spark

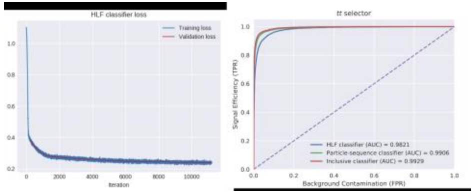
Data and models from Research

Input: labeled data and DL models

Feature engineering at scale

Hyperparameter optimization (Random/Grid search)

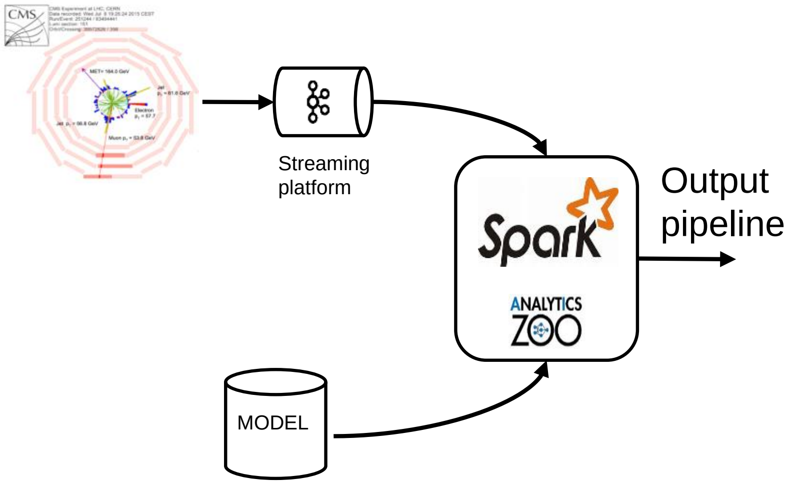
Distributed model training



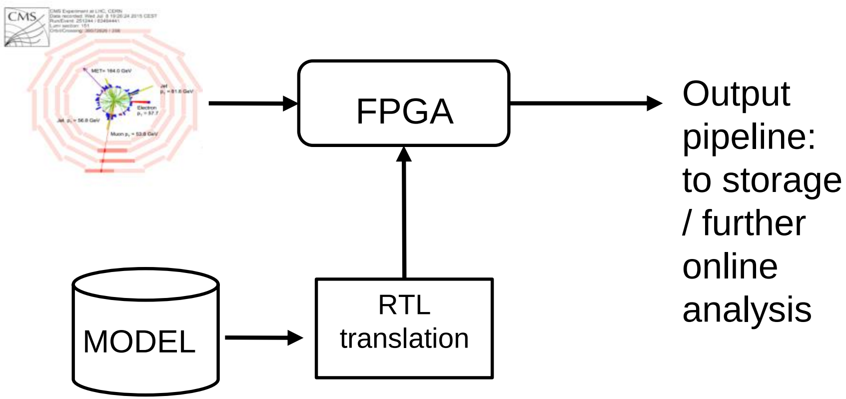
Output: particle selector model

Model Serving and Future Work

- Using Apache Kafka and Spark?



- FPGA serving DNN models



Summary

- The use case developed addresses the needs for higher efficiency in event filtering at LHC experiments
- 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
- Continuous evolution and improvements of DL at scale
  - Data preparation and scalable distributed training are key

Acknowledgments

- Matteo Migliorini, Marco Zanetti, Riccardo Castellotti, Michał Bień, Viktor Khristenko, CERN Spark and Hadoop service, CERN openlab
- 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
  - Analytics Zoo: https://github.com/intel-analytics/analytics-zoo
  - BigDL: https://software.intel.com/bigdl

References:

- 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

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