Basic Physics Analysis Implemented using Apache Spark

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Motivations and Scope

- Context: Spark service at CERN
- Recent work on implementing example analyses using PySpark on Jupyter notebooks
  - Blog: Can High Energy Physics Analysis Profit from Apache Spark APIs? https://db-blog.web.cern.ch/node/186

- I will mix an intro to Spark with notebooks examples
- Final thoughts on what I believe works OK with this approach and what needs improvements
- Not a goal: compete with state-of-the art software for analysis

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Apache Spark Adoption

- Who is using Spark, how, and why?
- Databricks

  - They sell a cloud-based analytics platform, centered around Spark
    - Development in the Spark ecosystem (Data Lakehouse, MLFlow)
    - They also have custom Spark improvements
  - Top contributors and drivers of the open-source development
- Cloud vendors
  - All offer user-facing “Big Data” platforms, typically including Spark
- Many tech giants use it internally
  - Facebook, Apple, MS, Baidu, Netflix, etc
  - Some contribute back to Spark development (Apache Spark PMCs)

Spark @ CERN

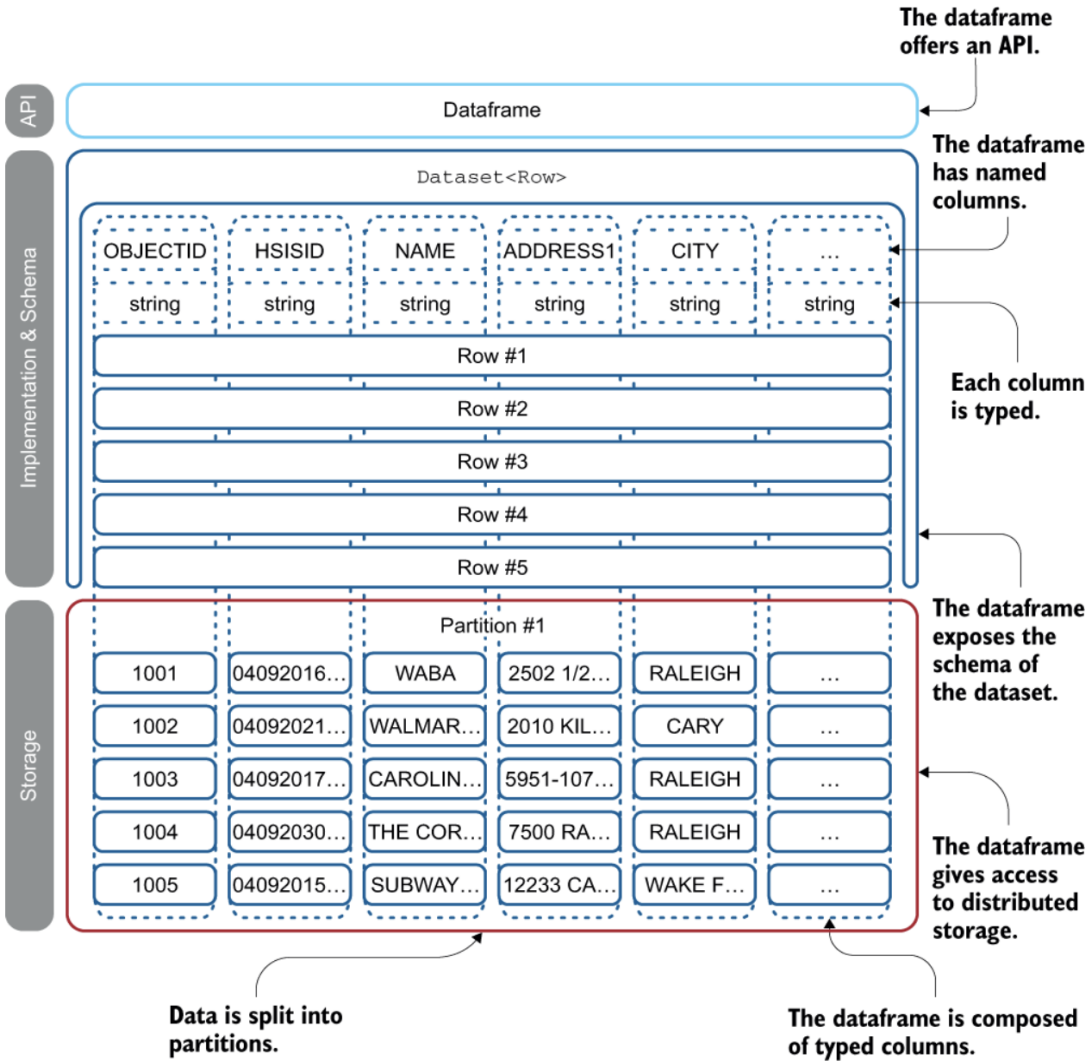
- Key component of the Hadoop platforms.
  - IT monitoring, IT security
  - Experiments computing data (e.g. reports for the Rucio project)
  - Physics: RDataFrame, CMS Spark, CMS Muon POG
- We also provide Spark on Kubernetes clusters
- User-access
  - Notebooks, often via SWAN. Some use of Spark on R
  - Batch jobs: Python, Scala, Java
- NXCals platform
  - Critical and large (~PBs) logging system for the accelerator complex
  - Platform based on Hadoop, API based on Spark

Demo 1

- Can Apache Spark run basic physics analysis?
- Let’s start with a “Hello World!” example

- Dimuon mass spectrum analysis at https://github.com/LucaCanali/Miscellaneous/tree/master/Spark_Physics

Main Data Abstraction: Spark DataFrames



- DataFrame is a table-like abstraction
  - similar to Pandas DF
- Handles data with a schema
- DFs are partitioned and immutable
  - enables parallel execution
  - and fault tolerance at scale

Figure from "Spark in action", Jean-Georges Perrin, Manning, 2020

DataFrame API Basics

- Selections and projection are easily scalable
- Filter operations naturally fit with the

```
# Apply filters to the input data
# - select only events with 2 muons
# - select only events where the 2 muons have opposite charge

df_muons = df_muons.filter("nMuon == 2").filter("Muon_charge[0] != Muon_charge[1]")
```

-

```
df_with_dimuonmass = df_muons.selectExpr("""
    sqrt(2 * Muon_pt[0] * Muon_pt[1] *
            ( cosh(Muon_eta[0] - Muon_eta[1]) - cos(Muon_phi[0] - Muon_phi[1]) )
        ) as Dimuon_mass""")
```

Histograms with the DataFrame API

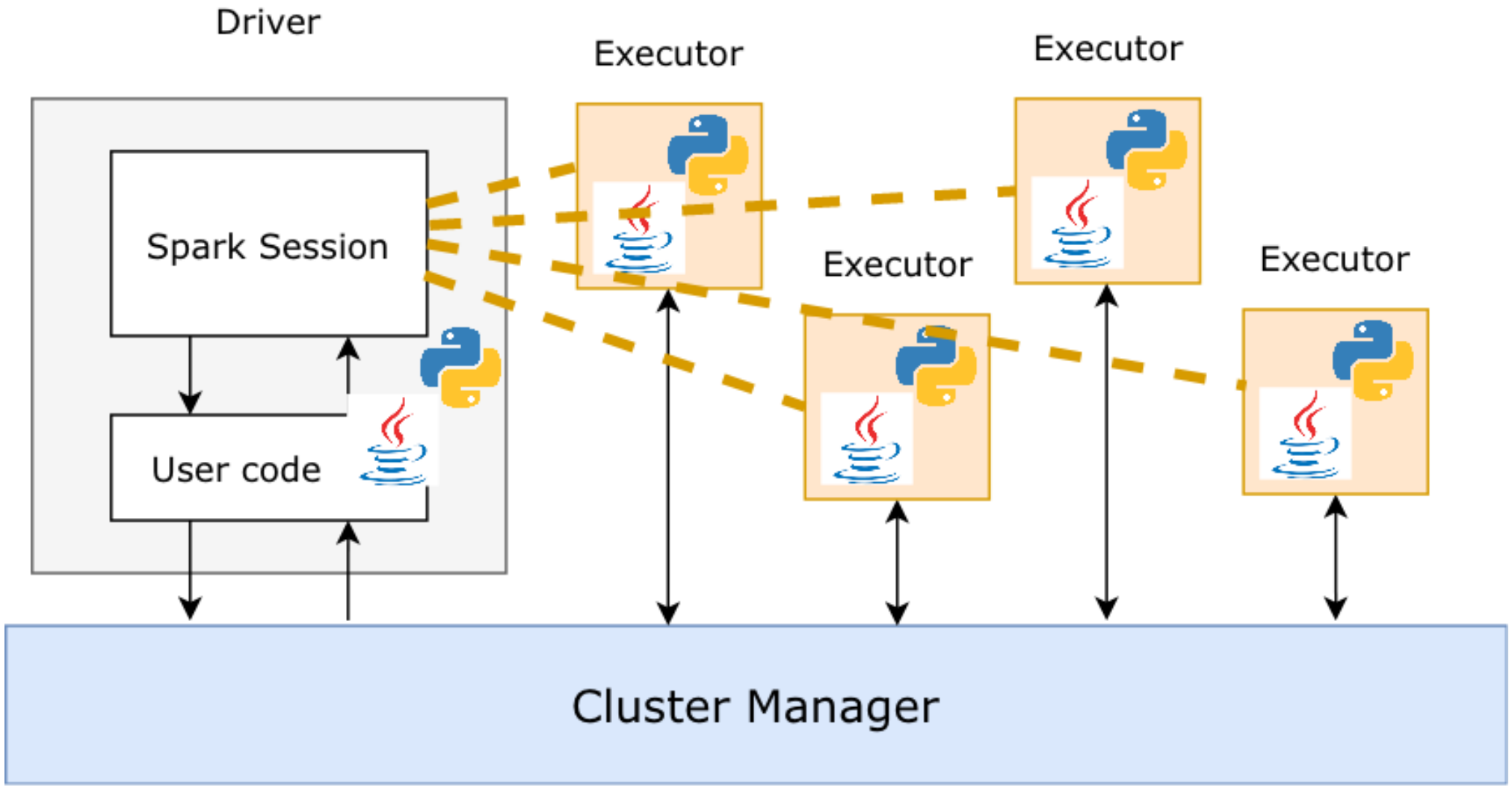
- Histograms are generated using Spark DataFrame API
  - Data aggregation/shuffle with Spark, can run at scale

```
from sparkhistogram import computeHistogram

# histogram parameters
min_val = 0.25
max_val = 300
num_bins = 30000

# use the helper function computeHistogram in the package sparkhistogram
histogram_data = computeHistogram(df_with_dimuonmass, "Dimuon_mass", min_val, max_val, num_bins)
```

How Spark Runs Jobs at Scale



Apache Spark Ecosystem

Use cases

Data analysis | Streaming Applications | Machine Learning | Graph Processing

Clusters

Laptop | Hadoop YARN | Kubernetes | Standalone

SQL, Python, Scala, Java, R

Libraries

SparkSQL DataFrames | Spark Streaming | MLlib | GraphX

Spark Core engine

Data formats

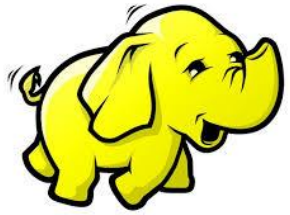
CSV | JSON | Parquet | Avro | ROOT

Storage

Hadoop | EOS | RDBMS | Streaming data | Cloud (S3...) | Other data sources

Apache Spark Clusters at CERN

- Spark running on clusters:
  - YARN/Hadoop -> established, use with HDFS storage
  - Spark on Kubernetes -> recommended when using EOS or S3 (cloud model)



Accelerator logging (part of LHC infrastructure)	Hadoop - YARN - 41 nodes (Cores - 1800, Mem - 18 TB, Storage – 13 PB)
General Purpose	Hadoop - YARN, 58 nodes (Cores – 2.6k, Mem – 30 TB, Storage – 21 PB)
Cloud containers	Kubernetes on Openstack VMs, Cores - 270, Mem – 2 TB Storage: remote HDFS or custom storage (CERN EOS, for physics data, S3 on Ceph also available). Note: GPU resources available.

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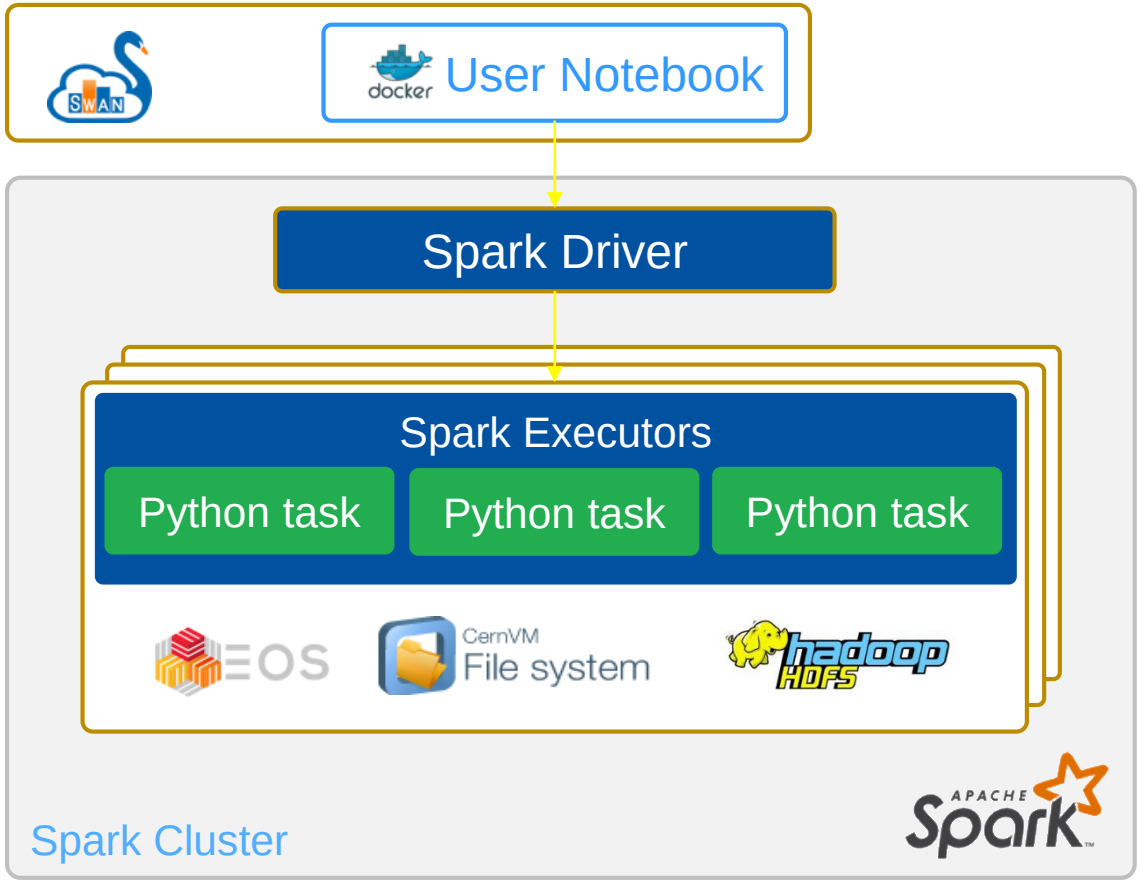
SWAN Integration with Apache Spark

- SWAN service: https://swan.web.cern.ch/swan/
  - Notebooks for web-based analysis
- Integrated with CERN Spark Clusters
  - Reduces configuration complexity for users
- CERN software environment
  - Software from CVMFS
- Graphical Jupyter extensions developed
  - Spark Connector
  - Spark Monitor
- Access to Spark Clusters
  - NXCals: – Dedicated cluster for accelerator logging
  - Analytix: – General purpose YARN cluster
  - Cloud Containers: – General purpose Kubernetes cluster
  - Storage access: HDFS, EOS, S3



Example 2

- Dimuon mass spectrum analysis on a cluster:

https://github.com/LucaCanali/Miscellaneous/tree/master/Spark_Physics

Spark can Handle Complex Schemas

- Example of complex schema for HEP

```
schema = "event LONG, HLT struct<flag1:boolean, flag2:boolean>, muons
ARRAY<STRUCT<pt:FLOAT, eta:FLOAT, phi:FLOAT, mass:FLOAT>>"

df.printSchema()

 |-- event: long (nullable = true)
 |-- HLT: struct (nullable = true)
 |    |-- flag1: boolean (nullable = true)
 |    |-- flag2: boolean (nullable = true)
 |-- muons: array (nullable = true)
 |    |-- element: struct (containsNull = true)
 |    |    |-- pt: float (nullable = true)
 |    |    |-- eta: float (nullable = true)
 |    |    |-- phi: float (nullable = true)
 |    |    |-- mass: float (nullable = true)
```

Handling Arrays

- Nested data is hard to handle
  - Does not fit naturally to DataFrame and SQL operations
- Available solutions in Spark
  - Array functions
    - Several available, example: array_min, array_sort, array_zip, …
  - “Explode” function
    - Transforms array values into DataFrame rows
  - Higher order functions
    - Process map/filter/aggregate on arrays elements
  - UDF: User-defined functions
    - General solution.
    - Spark UDF can be in Python or Scala

Demo 3

- HEP analysis benchmark notebooks

https://github.com/LucaCanali/Miscellaneous/tree/master/Spark_Physics

- Thanks to: https://iris-hep.org/projects/adl-benchmarks-index.html

Demo 4

- Outreach-style analysis
- Using Spark and Parquet: more familiar tools to data scientists outside HEP

- See example Higgs boson analysis at:

https://github.com/LucaCanali/Miscellaneous/tree/master/Spark_Physics

Lessons Learned and Wrap-up

What Spark Can Offer To HEP

- Spark DataFrame API:
  - Provide powerful abstractions and rich language(s)
    - Both for data preparation and analysis
  - Mature and an industry reference
  - Can handle complex schemas

- Run DataFrame locally and at scale using distributed computing
  - Runs on clusters and cloud (YARN/Hadoop, Kubernetes)
  - HPC and batch: can run Spark stand-alone (requires extra integration work)

- Integration with a large ecosystem
  - File formats: Parquet, csv, ROOT, …
  - Storage systems: HDFS, S3, EOS, ...
  - External systems: databases, elastic search, streaming, etc

Performance Gap

- Apache Spark Performance
  - Identified several areas of improvement for Apache Spark (3.3)
- Python UDF performance
  - Sending data to Python workers has been improved but still slow
- Spark functions
  - Higher order functions performance for array processing need improvements
  - More array functions and functions for Lorentz vector processing?
- Spark engine
  - Apache Spark does not (yet) have vectorized execution
  - State-of-the-art HEP tools have large parts running native code vs. Spark is currently mostly Scala and Java code running on the JVM (JIT compiled).

Open Questions: Data Formats

- ROOT data format ingestion is not optimized for Spark
  - It's a hard job with limited resources
  - Kudos to Andrew for Laurelin library + uproot team
- Apache Parquet and ORC
  - Optimized reader for Spark, supported by a large community
- The flatter the data the better
  - Data in nanoAOD format already much easier to process with Spark than deeply nested AOD

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Plans and Future Work

- Gather feedback
- Develop further examples and benchmarks
  - Trailing on work done with Coffea/Awkward array and with ROOT/RDataFrame
- Piggyback on Apache Spark improvements
  - Spark is still improving quite fast
- Work with community (HEP and Spark)
  - We noticed some interest by Apache Spark committers on understanding HEP use cases
  - Occasionally work together, as in the case of arrow UDF, also currently open SPARK-34265 and SPARK-38098
  - Some physicists also interested in trying out Spark ?

References + Acknowledgments

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• Evaluating Query Languages and Systems for High-Energy Physics Data, Dan Graur, Ingo Müller, Mason Proffitt, Ghislain Fourny, Gordon T. Watts, Gustavo Alonso, Proc. VLDB Endow., Vol 15, Issue 2 (2021).

• Get started with Spark at CERN: https://hadoop-user-guide.web.cern.ch/

• Thanks:
  • to the teams in the IT Hadoop, Spark and streaming service, and in the SWAN service, in particular to Riccardo Castellotti.
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