CIML Summer Institute 2022
Scalable Machine Learning

SDSC SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego

Scalable Machine Learning Agenda

8:00 - 8:05 – Welcome
8:05 - 9:05 – Introduction to Singularity
9:05 - 10:50 – CONDA & Jupyter on Expanse
10:50 - 11:20 – Break/Lunch
11:20 - 11:35 – Machine Learning Overview
11:35 - 12:15 – R on HPC
12:15 - 12:25 – Break
12:25 - 2:05 – Spark

Spark

Mai H. Nguyen, Ph.D.

Spark Topics

- **Spark**
  - History & Design Goals
  - RDDs
  - DataFrames
  - Spark Architecture
  - Spark API
  - Spark Core & Libraries
- **Spark Hands-On**
  - Scaling
  - Cluster Analysis
- **SparkR**

SPARK

- **Computing platform for distributed computing**
  - Built-in parallelism & fault-tolerance on commodity cluster
  - Provides interactive querying, iterative analytics, streaming processing
  - Goals: speed, ease of use, generality, unified platform
- **History**
  - Research project began in 2009 at UC Berkeley's AMPlab
  - Paper published in 2010
  - Contributed to Apache Software Foundation in 2013
  - Commercial version by Databricks

SPARK

- Goals: **speed**, ease of use, generality, unified platform
- In-memory processing
  - Exploits distributed memory to cache data
  - Intermediate results written to memory whenever possible
- How does Spark manage data in distributed system?

RESILIENT DISTRIBUTED DATASETS (RDDs)

- Spark central concept
  - Abstraction of data as distributed collection of objects

- Data abstraction
  - Resilient Distributed Datasets (RDDs)
  - Programming construct for storing data
  - Spark uses RDDs to distribute data and computations across nodes in cluster

RDD

- Resilient Distributed **Dataset**
  - Collection of data
    - From files in local filesystem (text, JSON, etc.)
    - From data store (HDFS, RDBMS, NoSQL, etc.)
    - Created from another RDD
- Resilient **Distributed** Dataset
  - Data is divided into partitions
  - Partitions are distributed across nodes in cluster
- **Resilient** Distributed Dataset
  - Provides resilience (e.g., fault tolerance) to failures
  - History of operations performed on each partition is tracked to provide lineage-based fault tolerance
- All provided automatically by Spark engine

SPARK CONTEXT

- Spark Context
  - Entry point to Spark engine
  - Provides way to create RDDs

```
from pyspark import SparkContext, SparkConf

conf = SparkConf()\
   .setAppName("RDD Example") \
   .config("config.option","config.value")
sc = SparkContext(conf=conf)
```

- SparkContext: connection to Spark engine
- SparkConf: configuration parameters for application

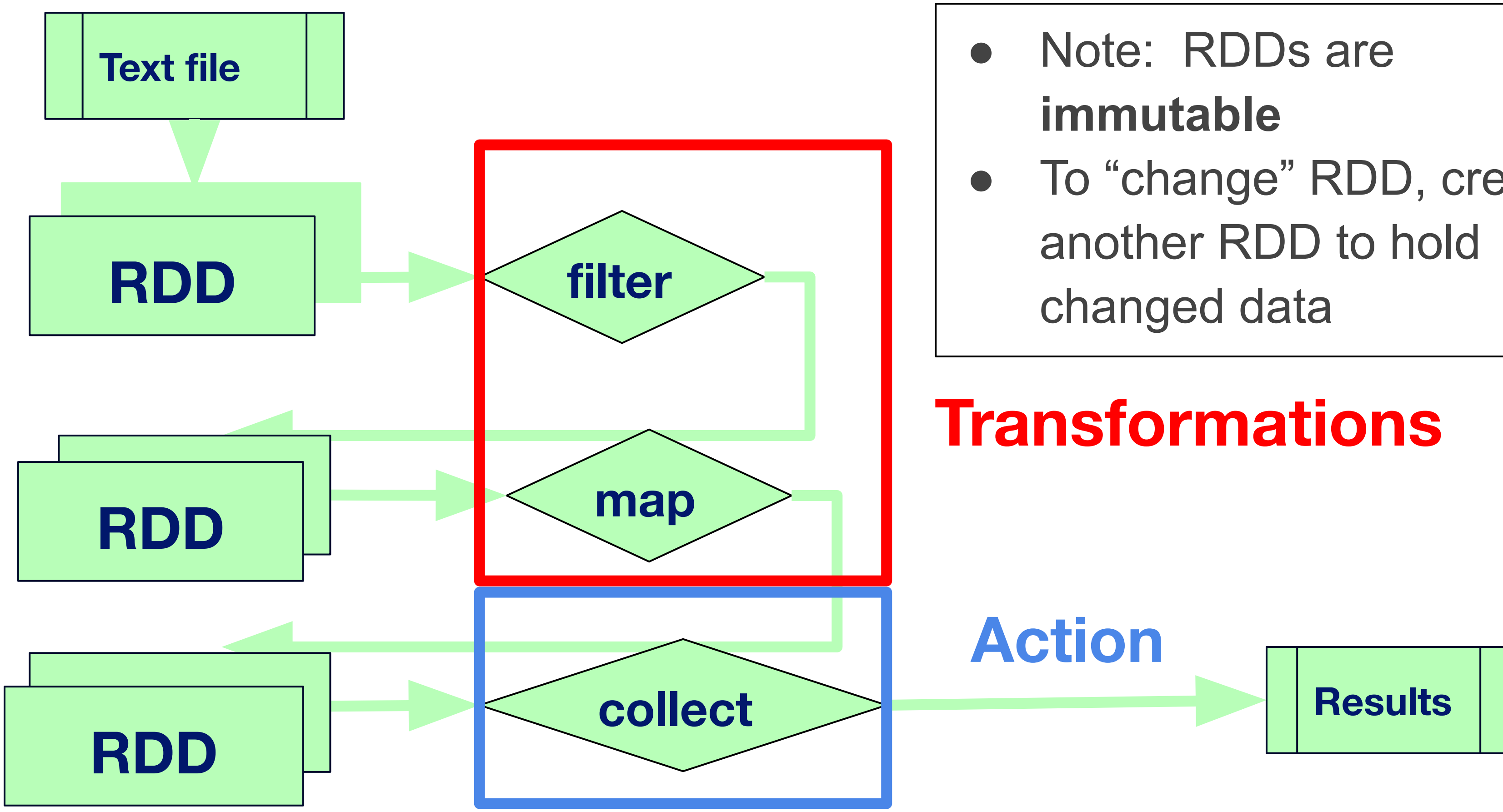
CREATING RDDs

- Read data from files in local filesystem (text, JSON, etc.)
  - lines = sc.textFile("inputfile.txt")
- Data read in from data store (HDFS, RDBMS, NoSQL, etc.)
  - lines = sc.textFile("hdfs://<path>/inputfile.txt")
- Generate data
  - numbers = sc.parallelize(range(100),3)
    - Divide data into 3 partitions
- Created by transforming another RDD
  - newLines = lines.filter(lambda s: "Spark" in s)

PROCESSING RDDs

- RDDs can be processed using 2 types of operations
  - **Transformation**: Creates new RDD from existing RDD
  - **Action**: Runs computation(s) on RDD and returns value

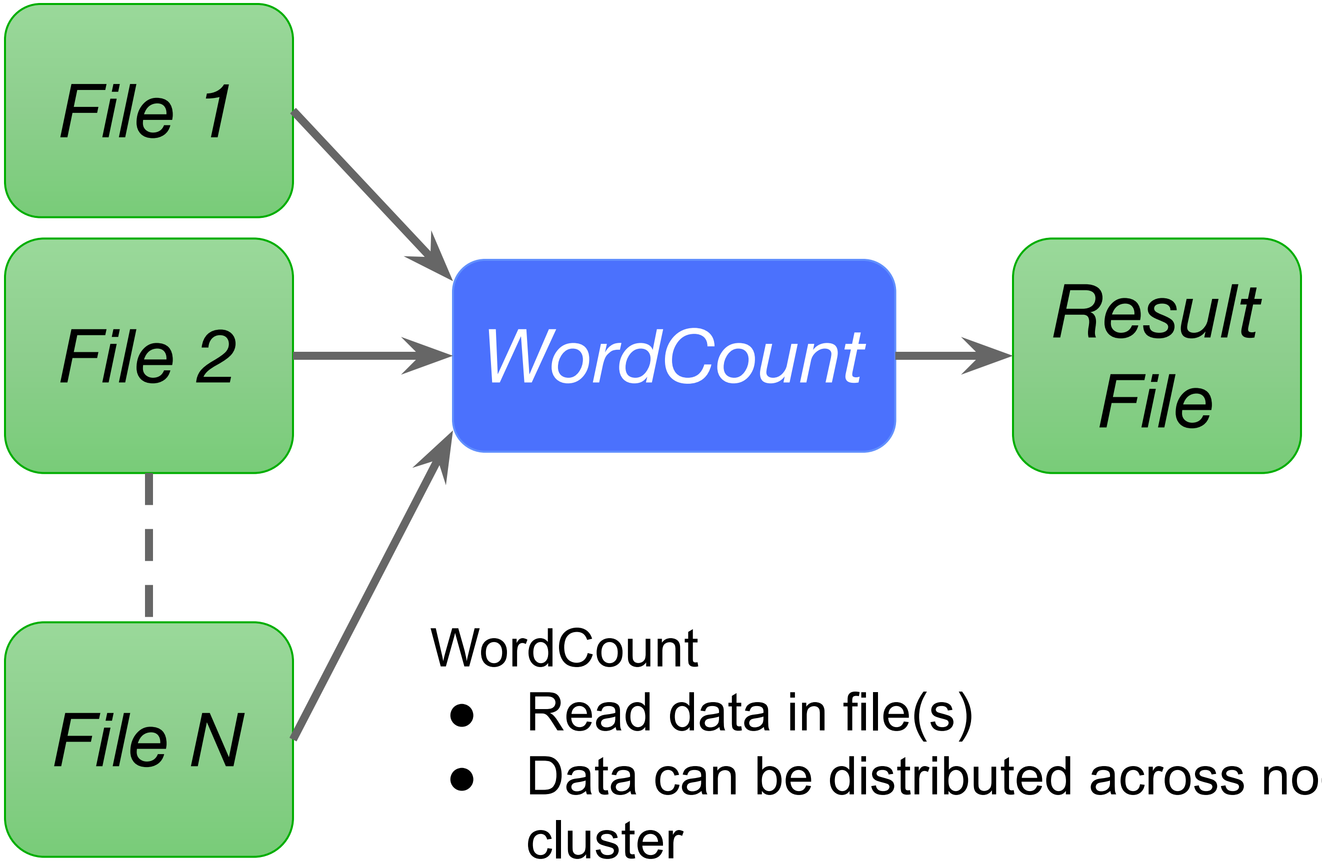
- Note: RDDs are **immutable**
- To “change” RDD, create another RDD to hold changed data



LAZY EVALUATION

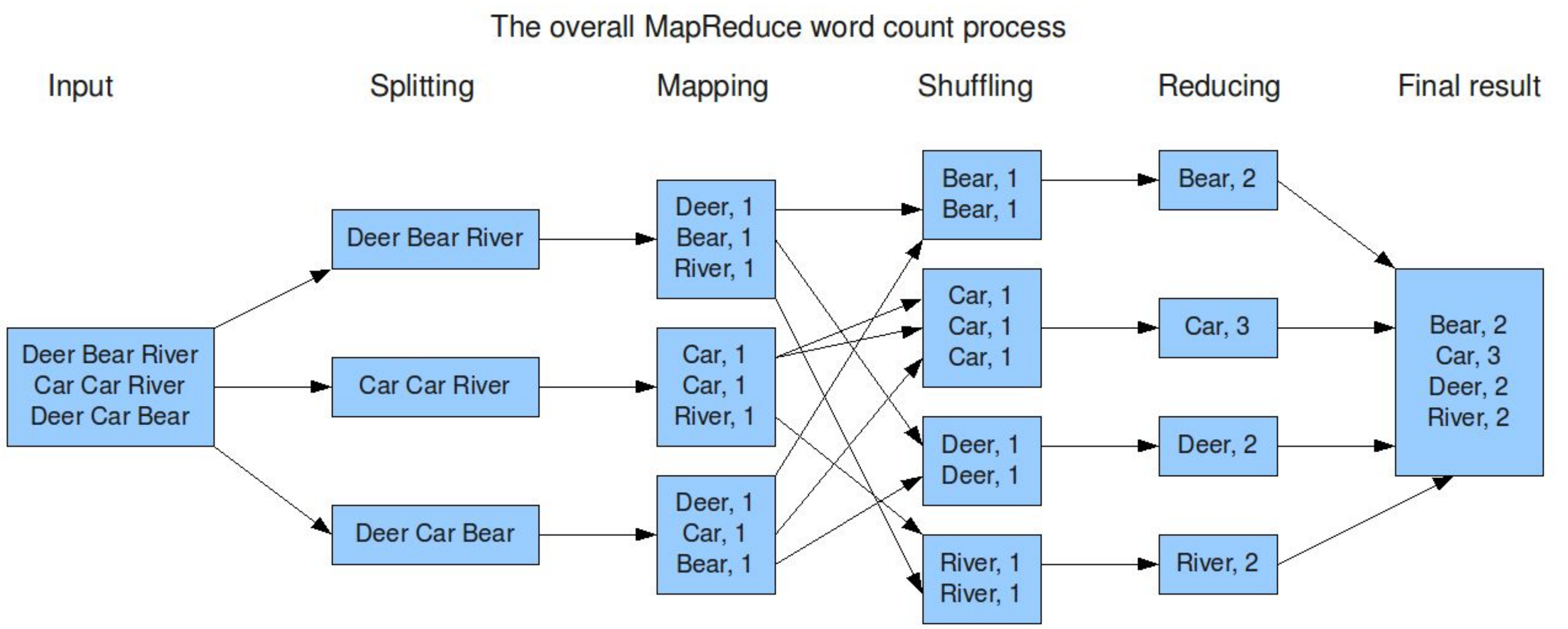
- Transformations on RDDs have **lazy evaluation**
  - Transformations are not immediately processed
  - Plan of operations is built
- Operations executed when **action** is performed
  - i.e., actions force computation
- Allows for optimizations in generating physical plan
- Example:
  - filtered = strings.filter(strings.value.contains(“Spark”))
    - Nothing is returned
  - filtered.count()
    - ‘filter’ is performed, and count is returned

WordCount



WordCount
- Read data in file(s)
- Data can be distributed across nodes in cluster
- Count number of occurrences of each word

WordCount



https://www.todaysoftmag.com/article/1358/hadoop-mapreduce-deep-diving-and-tuning

Data is partitioned across nodes

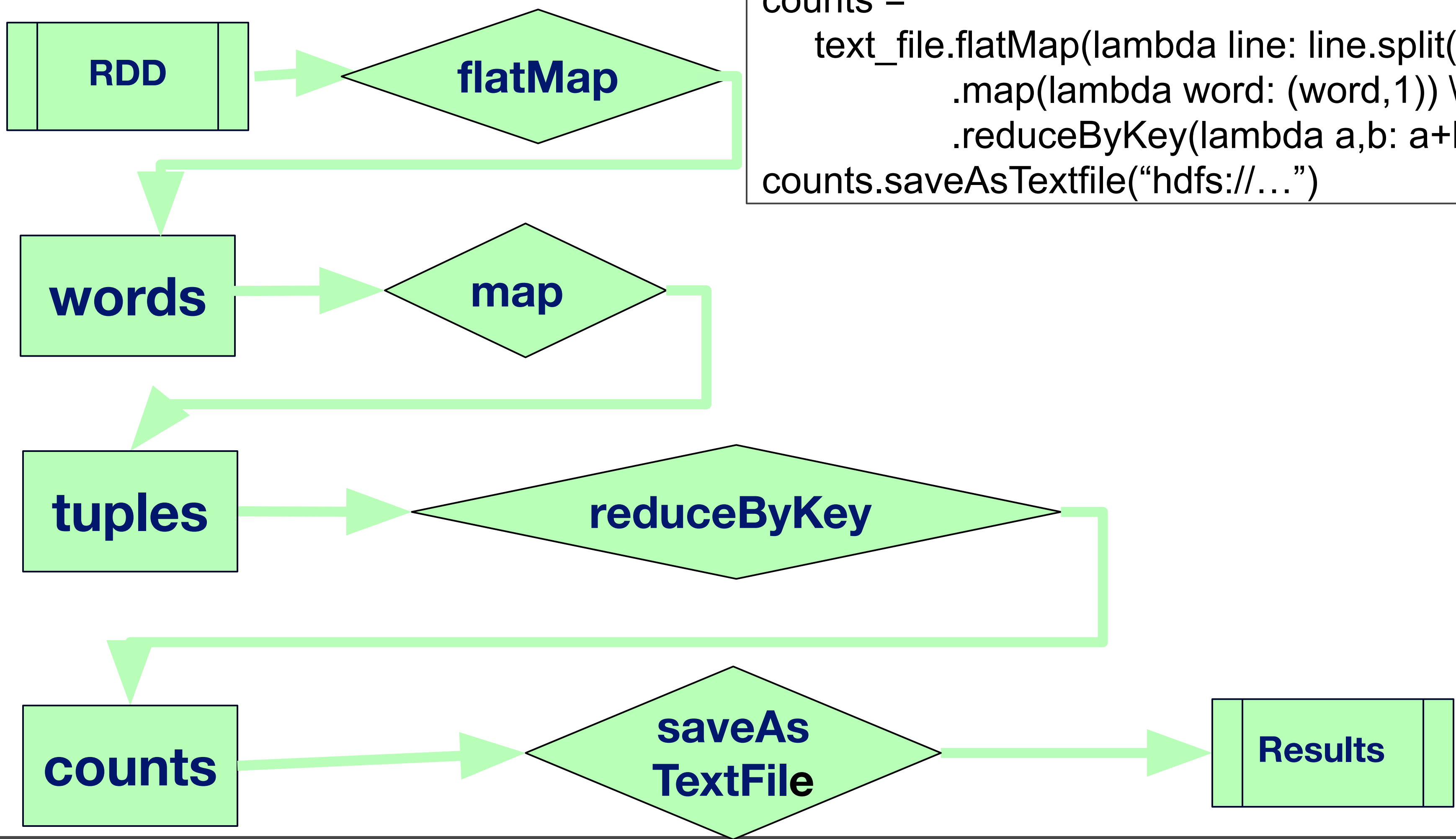
Map generates key-value pairs

Pairs with same key moved to same node

Reduce sums values for each key

WordCount (RDD)

```
text_file = sc.textFile("hdfs://..")
counts =
    text_file.flatMap(lambda line: line.split(" ")) \
                 .map(lambda word: (word,1)) \
                 .reduceByKey(lambda a,b: a+b)
counts.saveAsTextfile("hdfs://…")
```



DATAFRAMES & DATASETS

- **Extensions to RDDs**
  - Higher-level abstractions
  - Improved performance
  - Better scalability
- **Can convert to/from RDDs and use with RDDs**

DATAFRAMES & DATASETS

DataFrame

- Lazy evaluation
- Immutable
- Data organized as collection of Rows
- No static type checking
- APIs in Java, Scala, Python, R

DataSet

- Lazy evaluation
- Immutable
- Data organized as collection of Rows
- Static type checking
- APIs in Java and Scala

USING DATAFRAMES

- Spark Session
    - Entry point to Spark engine
    - Note that SparkContext is now **SparkSession**

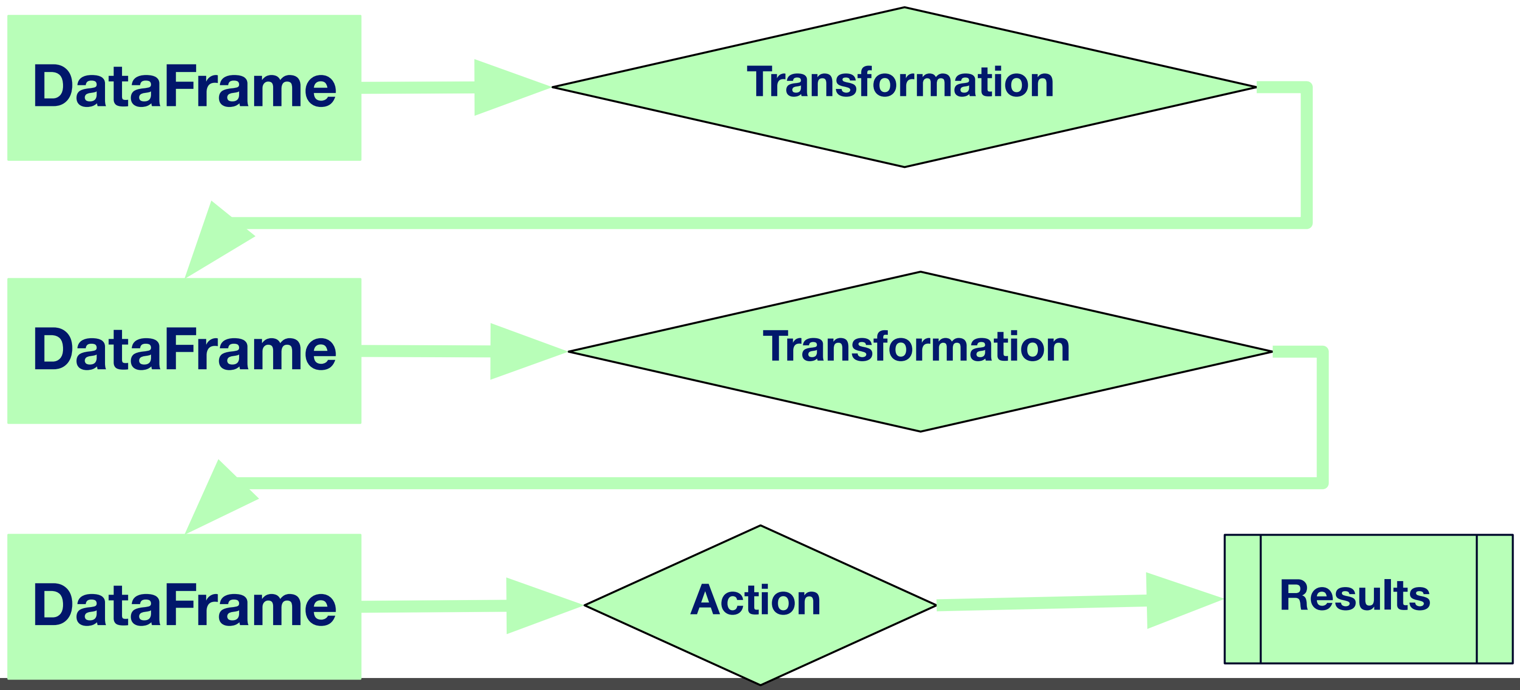
```
from pyspark import SparkSession, SparkConf

conf = SparkConf \
   .setAll \
   ([("spark.app.name","DataFrame Example") \
   ("config.option","config.value")])

spark =
   SparkSession.builder.config(conf=conf)\
                .getOrCreate()
```

CREATING DATAFRAMES

- Read data from files in local filesystem (text, JSON, etc.)
  - df = spark.read.csv(“data.csv”, header=”True”)
- Data read in from data store (HDFS, RDBMS, NoSQL, etc.)
  - df = spark.read.csv(“hdfs:///<path>/data.csv”)
- Generate data
  - empl_0 = Row(id=”123”, name=”John”)
  - empl_1 = Row(id=”456”, name=”Mary”)
  - employees = [empl_0, empl_1]
  - df = spark.createDataFrame(employees)
- Created by transforming another DataFrame
  - filter_df = df.filter(col(“name”)==”Mary”))

DATAFRAME TRANSFORMATIONS & ACTIONS

- Similar to RDDs, DataFrames can be processed using transformations and actions
- Transformations on DataFrames also have lazy evaluation
- Operations executed when action is performed



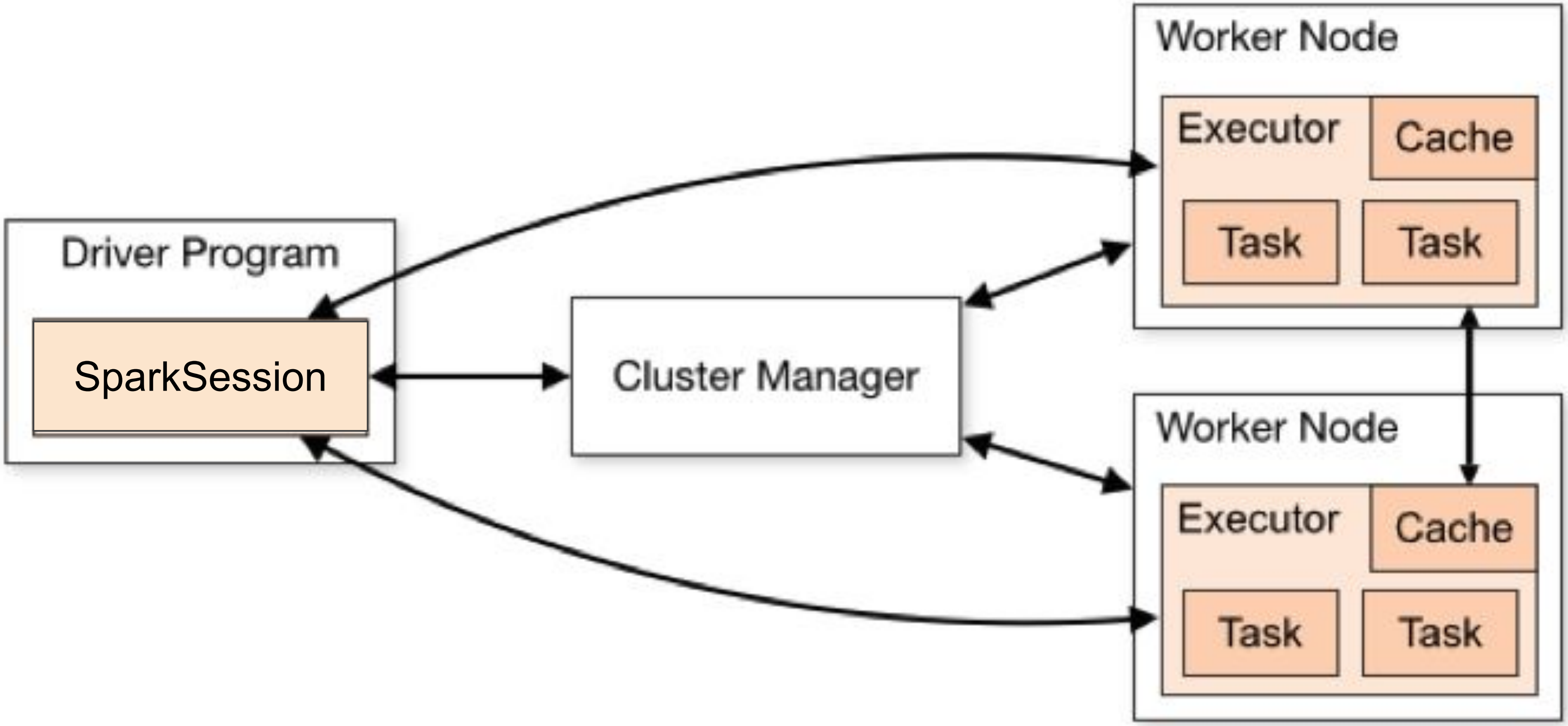
DATA PERSISTENCE

- Persist data through caching
  - Data is stored in memory to avoid re-computing
- Can specify different storage levels
  - In memory, on disk, serialized in memory, etc.
- Examples
  - df.cache() – MEMORY_ONLY
  - df.persist(MEMORY_ONLY_SER) – Serialized in memory
  - df.unpersist() – Remove from cache

SPARK PROGRAM STRUCTURE

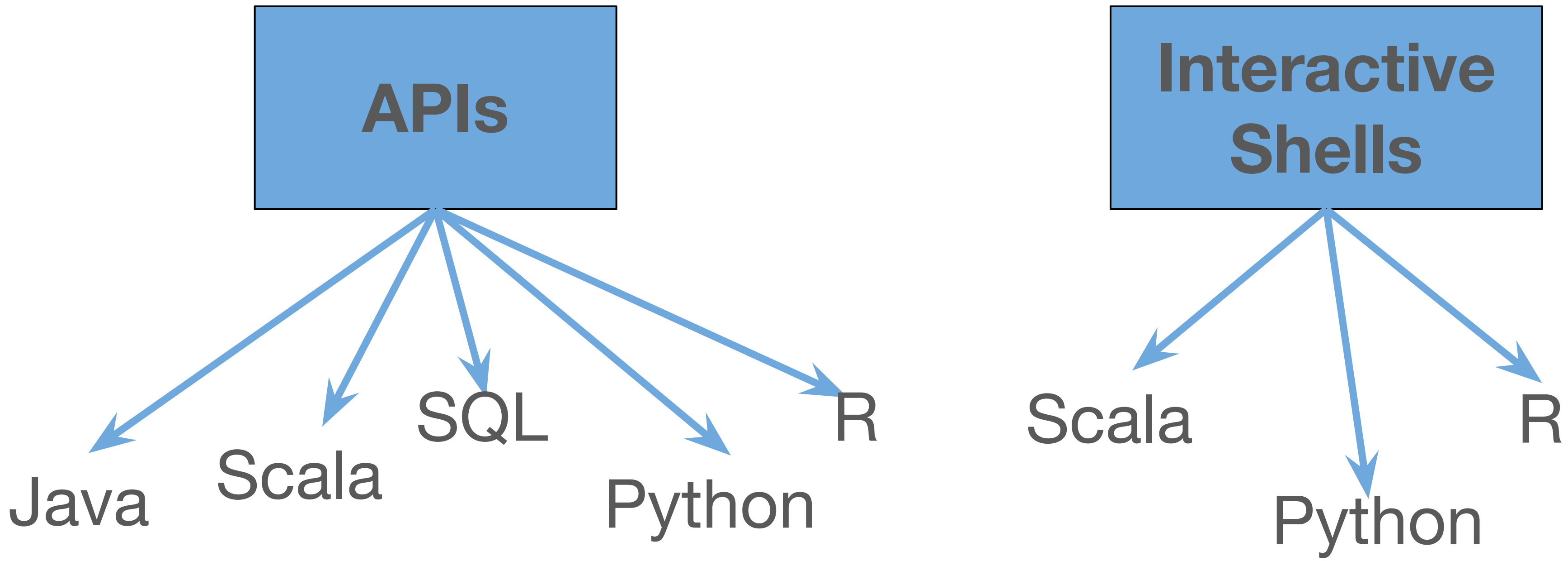
- **Start Spark session**
  - spark = SparkSession.builder.config(conf=conf).getOrCreate()
- **Create distributed dataset**
  - df = spark.read.csv(“data.csv”,header=”True”)
- **Apply transformations**
  - new_df = df.filter(col(“dept”) == “Sales”)
- **Perform actions**
  - df.collect()
- **Stop Spark session**
  - spark.stop()

SPARK ARCHITECTURE



SPARK INTERFACE

Goals: speed, **ease of use**, generality, unified platform



RDD WORDCOUNT EXAMPLE IN SPARK

Spark RDD API available in Python, Scala, Java, and R

```
text_file = sc.textFile("hdfs://...")
counts = text_file.flatMap(lambda line: line.split(" ")) \
             .map(lambda word: (word, 1)) \
             .reduceByKey(lambda a, b: a + b)
counts.saveAsTextFile("hdfs://...")
```

```
val textFile = sc.textFile("hdfs://...")
val counts = textFile.flatMap(line => line.split(" "))
                 .map(word => (word, 1))
                 .reduceByKey(_ + _)
counts.saveAsTextFile("hdfs://...")
```

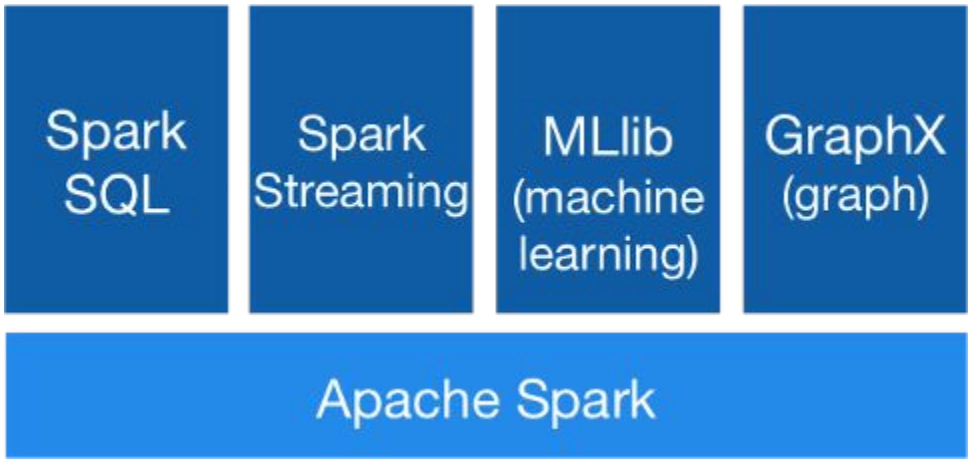
```
JavaRDD<String> textFile = sc.textFile("hdfs://...");
JavaPairRDD<String, Integer> counts = textFile
    .flatMap(s -> Arrays.asList(s.split(" ")).iterator())
    .mapToPair(word -> new Tuple2<>(word, 1))
    .reduceByKey((a, b) -> a + b);
counts.saveAsTextFile("hdfs://...");
```

SPARK - GENERALITY

- Goals: speed, ease of use, **generality,** unified platform
- Support for several data sources
  - Local file systems, HDFS, RDBMSs, MongoDB, Kafka, AWS S3, etc.
- Can run on various platforms
  - Hadoop, Kubernetes, cloud, standalone
- Support for multiple workloads
  - batch, streaming
  - machine learning, SQL, graph processing

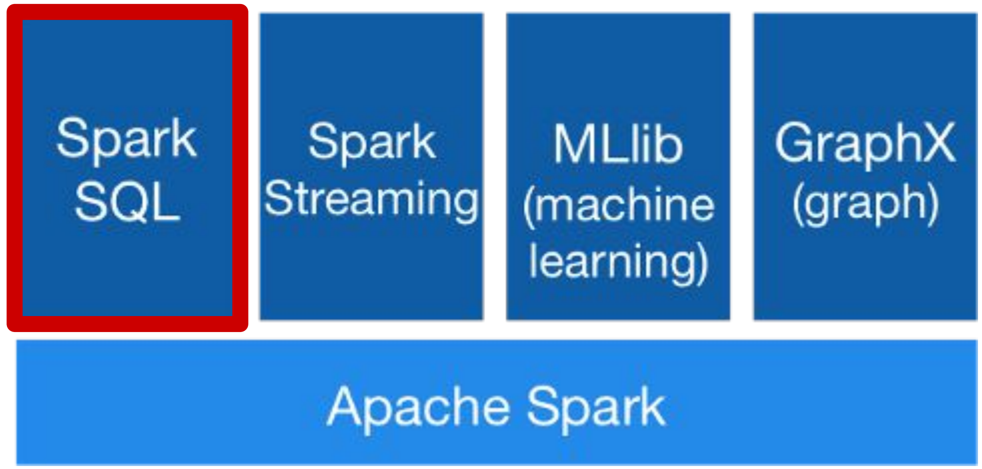
SPARK - UNIFIED PLATFORM

- Goals: speed, ease of use, generality**, unified platform**



- Provides unified platform for various analytics processing
- **Spark engine** provides core capabilities for distributed processing
- **Spark libraries** provide additional higher-level functionality for diverse workloads

SPARK SQL



- **Structured Data Processing**
  - Provides support for SQL and query processing
  - Structure of data and computations allow for efficient query plan can be constructed
  - Has APIs for SQL, Scala, Java, Python, and R
  - Generated underlying code is identical

SPARK SQL

- Execute SQL queries
  - SQL

```
spark.sql("SELECT max(count)
FROM flight_data").take(1)
```

  - PySpark

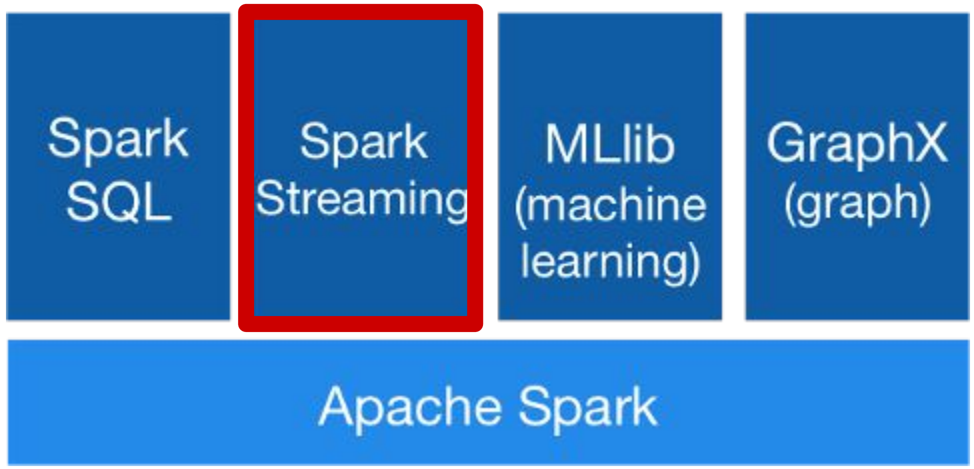
```
from pyspark.sql.functions import max
flight_data.select(max("count")).take(1)
```

SPARK SQL

- Integrate SQL queries with Spark commands

```
df = spark.sql ("SELECT * FROM Employees")
df.show(100)

num_employees =
  df.select("Age","Dept","Salary")
    .groupBy("Dept")
    .where(df.Salary > 80000)
    .count()
```

SPARK STREAMING



- **Streaming Data Processing**
  - Scalable processing for real-time analytics
  - Structured streaming
    - Data stream is divided into micro-batches of data
    - Same operations for static data can be used
  - Has APIs for Scala, Java, and Python

REAL-TIME ANALYTICS

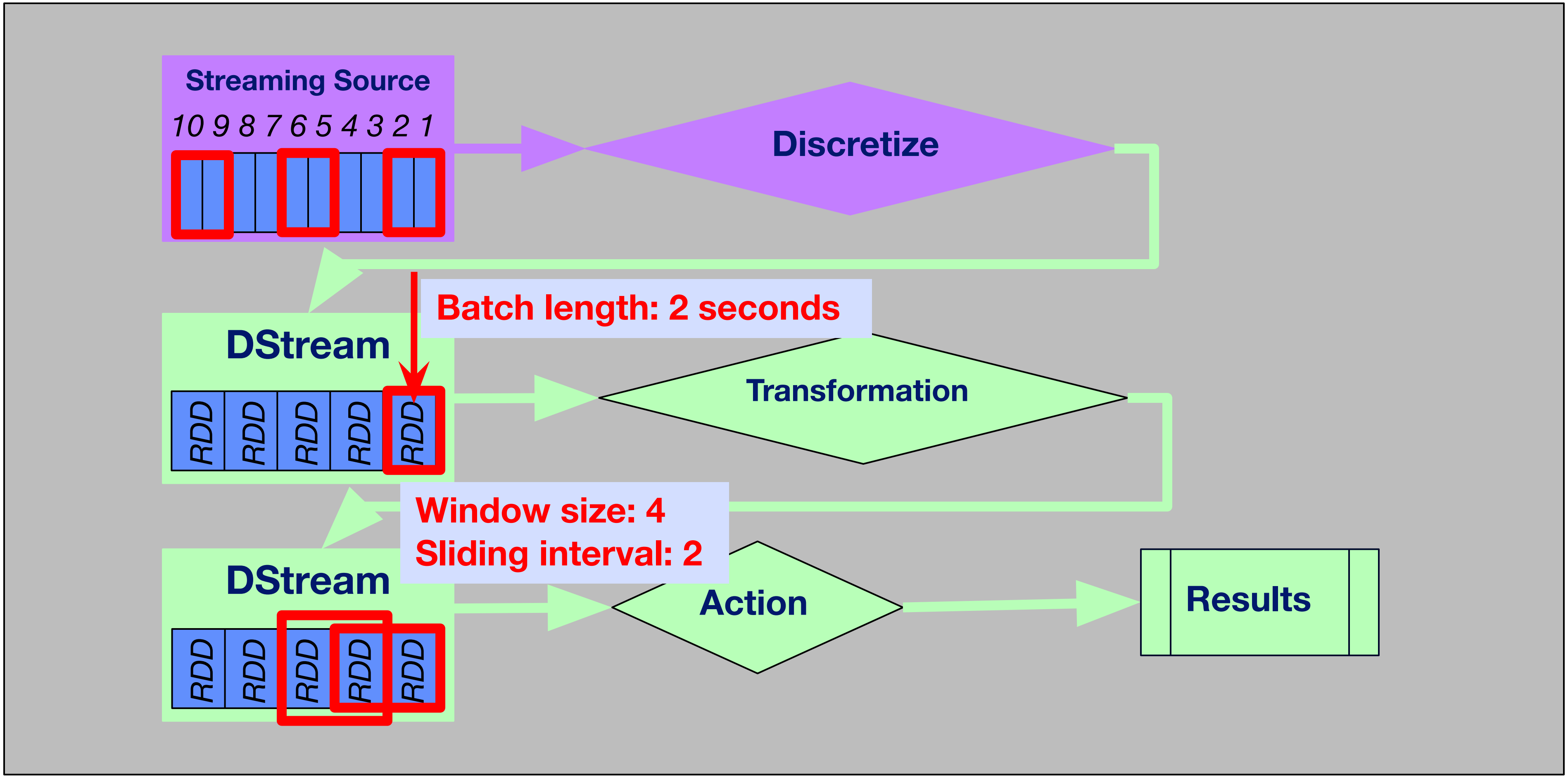
- (Near) Real-Time Analytics
  - Analysis and use of data as it enters system
- Examples
  - Identifying fraudulent credit card transaction at point-of-sale
  - Viewing orders as they happen for up-to-date inventory tracking and trend analysis
  - Understanding trending topics of tweets/news articles/etc.

SPARK STREAMING

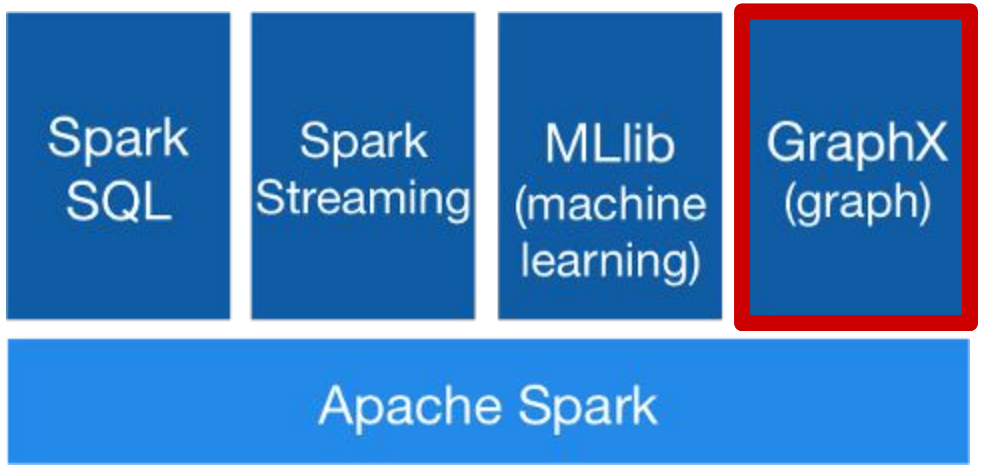
- Input data stream is divided into batches of data that are processed by Spark engine
- DStream: high-level abstraction
  - Implemented as sequence of RDDs
- Any Spark operation can be applied to DStreams

https://spark.apache.org/docs/latest/streaming-programming-guide.html

SPARK STREAMING



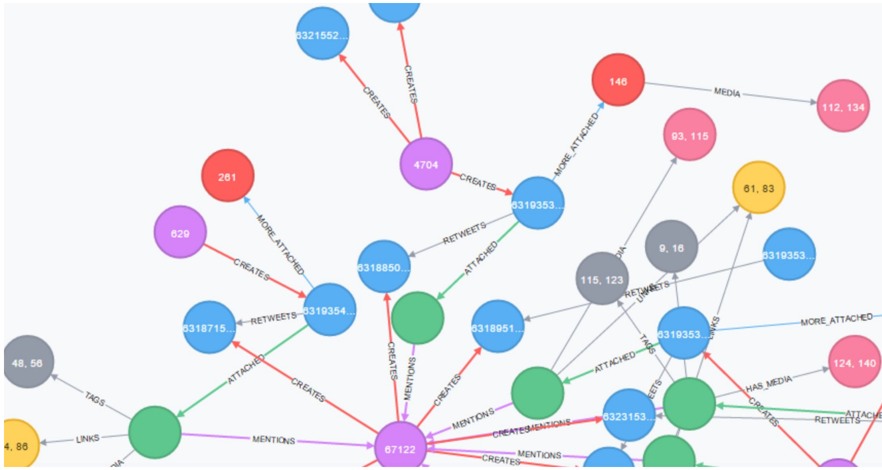
SPARK GRAPHX / GRAPHFRAMES



- **Graph Computation**
  - Distributed graph processing
  - Special structures for storing vertex and edge information & operations for manipulating graphs
  - GraphX (RDD-based) & GraphFrames (DF-based)
  - Has APIs in Scala, Java, Python (GraphFrames)

SPARK GRAPHX / GRAPHFRAMES

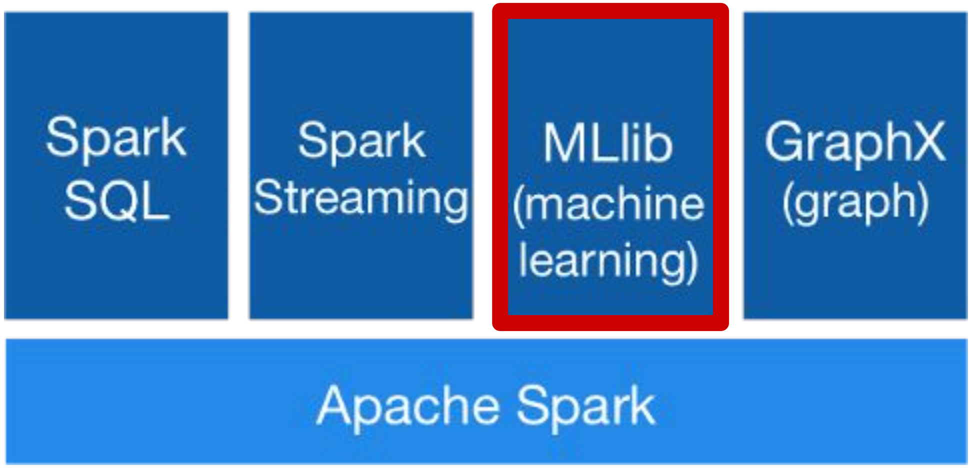
- **Graph analytics**
  - Analysis of relations among entities
- **Data represented as graph**
  - Entities are vertices
  - Relationships are edges
- **Example: Analyzing tweets**
  - Extract conversation threads
  - Find interacting groups
  - Find influencers in community



SPARK GRAPHX / GRAPHFRAMES

- Graph operators & algorithms
  - Connected Components
  - PageRank
  - Triangle Counting
  - Label Propagation Algorithm
  - Shortest Paths

SPARK MLLIB



- **Machine Learning**
  - Scalable machine learning library
  - Distributed implementations of machine learning algorithms and utilities
  - Has APIs for Scala, Java, Python, and R

SPARK MLLIB ALGORITHMS

- **Machine Learning**
  - Classification, regression, clustering, etc.
  - Evaluation metrics
- **Statistics**
  - Summary statistics, sampling, etc.
- **Utilities**
  - Dimensionality reduction, transformation, etc.
- **ML Pipelines**
  - Similar to scikit-learn

MLLIB EXAMPLE: STATISTICS

```
from pyspark.sql.functions import rand

# Generate random numbers
df = sqlContext.range(0,10)
       .withColumn("rand1", rand(seed=10))
       .withColumn("rand2", rand(seed=27))


# Show summary statistics
df.describe().show()


# Compute correlation
df.stat.corr("rand1","rand2")
```

MLLIB EXAMPLE: CLUSTER ANALYSIS

```
from pyspark.ml.clustering import KMeans

# Read and parse data
data = spark.read.csv("data.csv", header="true")


# k-means model for clustering
kmeans = Kmeans().setK(3).setSeed(123)
model  = kmeans.fit(data)
for centers in model.clusterCenters()
   print (centers)
```

MLLIB EXAMPLE: CLASSIFICATION

```
from pyspark.ml.classification import DecisionTreeClassifier

# Split data into train & test sets
trainDF,testDF = data.randomSplit([0.7,0.3],seed=123)

# Build model
dt = DecisionTreeClassifier(
          featuresCol='features',
          labelCol='label',
          predictionCol='prediction')
model = dt.fit(trainDF)

# Test model
predictions = model.transform(testDF)
```

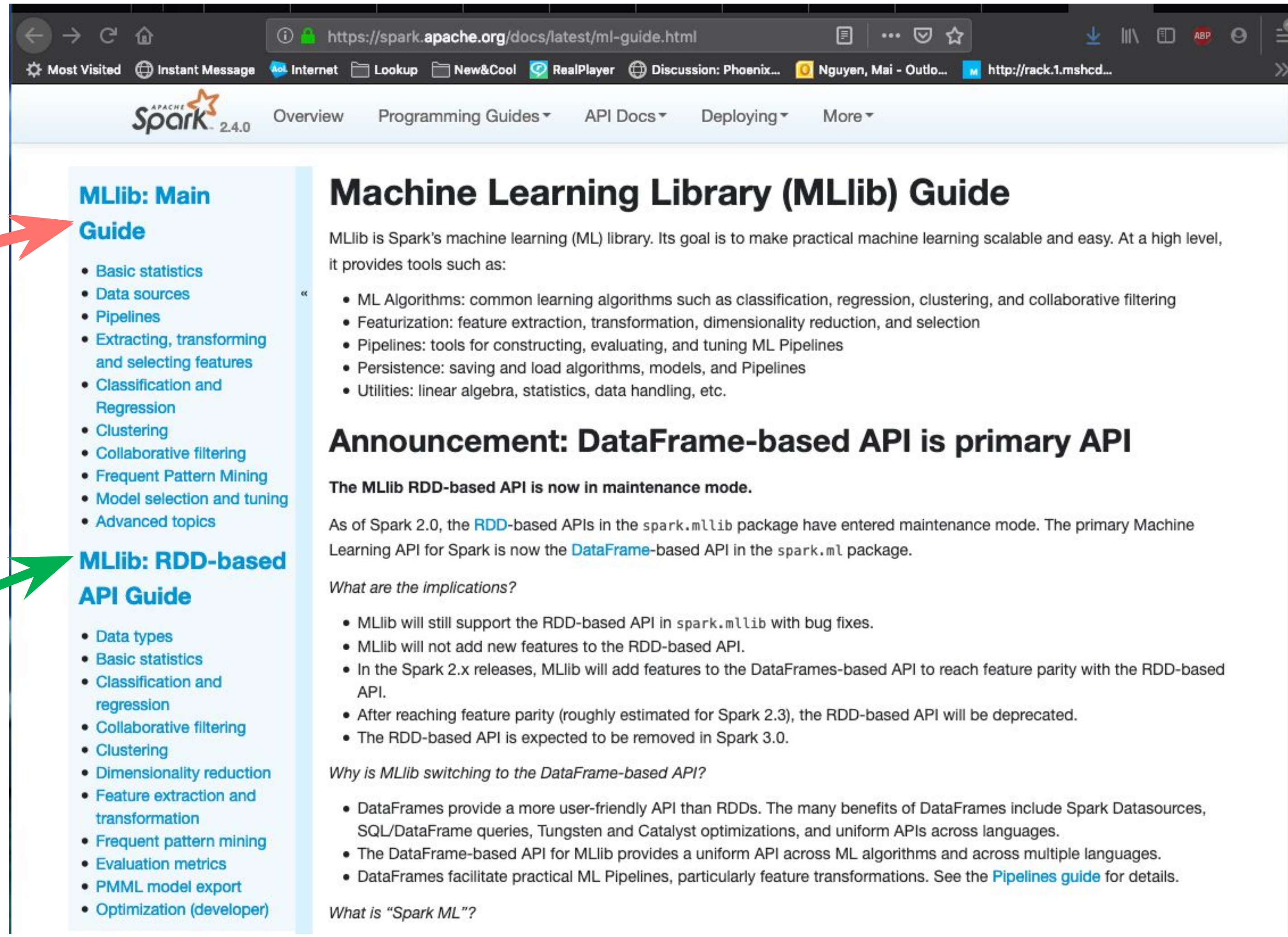
MLLIB LIBRARIES

ml

(DataFrame-based)

mllib

(RDD-based)


https://spark.apache.org/docs/latest/ml-guide.html

Spark 2.4.0 Overview Programming Guides API Docs Deploying More

MLlib: Main Guide

- Basic statistics
- Data sources
- Pipelines
- Extracting, transforming and selecting features
- Classification and Regression
- Clustering
- Collaborative filtering
- Frequent Pattern Mining
- Model selection and tuning
- Advanced topics

MLlib: RDD-based API Guide

- Data types
- Basic statistics
- Classification and regression
- Collaborative filtering
- Clustering
- Dimensionality reduction
- Feature extraction and transformation
- Frequent pattern mining
- Evaluation metrics
- PMML model export
- Optimization (developer)

Machine Learning Library (MLlib) Guide

MLlib is Spark's machine learning (ML) library. Its goal is to make practical machine learning scalable and easy. At a high level, it provides tools such as:

- ML Algorithms: common learning algorithms such as classification, regression, clustering, and collaborative filtering
- Featurization: feature extraction, transformation, dimensionality reduction, and selection
- Pipelines: tools for constructing, evaluating, and tuning ML Pipelines
- Persistence: saving and load algorithms, models, and Pipelines
- Utilities: linear algebra, statistics, data handling, etc.

Announcement: DataFrame-based API is primary API

The MLlib RDD-based API is now in maintenance mode.

As of Spark 2.0, the RDD-based APIs in the `spark.mllib` package have entered maintenance mode. The primary Machine Learning API for Spark is now the DataFrame-based API in the `spark.ml` package.

What are the implications?

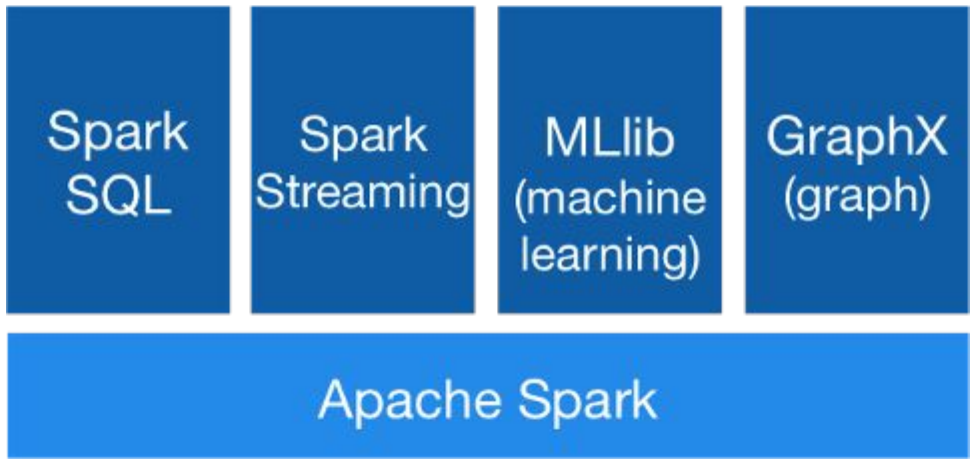
- MLlib will still support the RDD-based API in `spark.mllib` with bug fixes.
- MLlib will not add new features to the RDD-based API.
- In the Spark 2.x releases, MLlib will add features to the DataFrames-based API to reach feature parity with the RDD-based API.
- After reaching feature parity (roughly estimated for Spark 2.3), the RDD-based API will be deprecated.
- The RDD-based API is expected to be removed in Spark 3.0.

Why is MLlib switching to the DataFrame-based API?

- DataFrames provide a more user-friendly API than RDDs. The many benefits of DataFrames include Spark Datasources, SQL/DataFrame queries, Tungsten and Catalyst optimizations, and uniform APIs across languages.
- The DataFrame-based API for MLlib provides a uniform API across ML algorithms and across multiple languages.
- DataFrames facilitate practical ML Pipelines, particularly feature transformations. See the Pipelines guide for details.

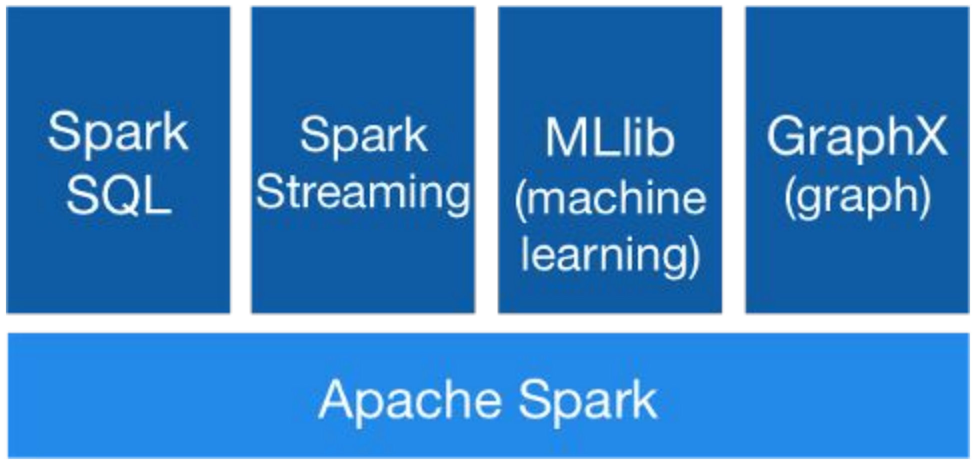
What is "Spark ML"?

SPARK LIBRARIES



- **Spark Libraries**
  - Use Spark engine as core
  - Extend functionality to particular applications
  - Third-party packages: https://spark-packages.org

SPARK



Goals: speed, ease of use, generality, unified platform