

Data Integration and Large-scale Analysis (DIA)

11 Distributed, Data-parallel Computation

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Announcements / Administrative Items



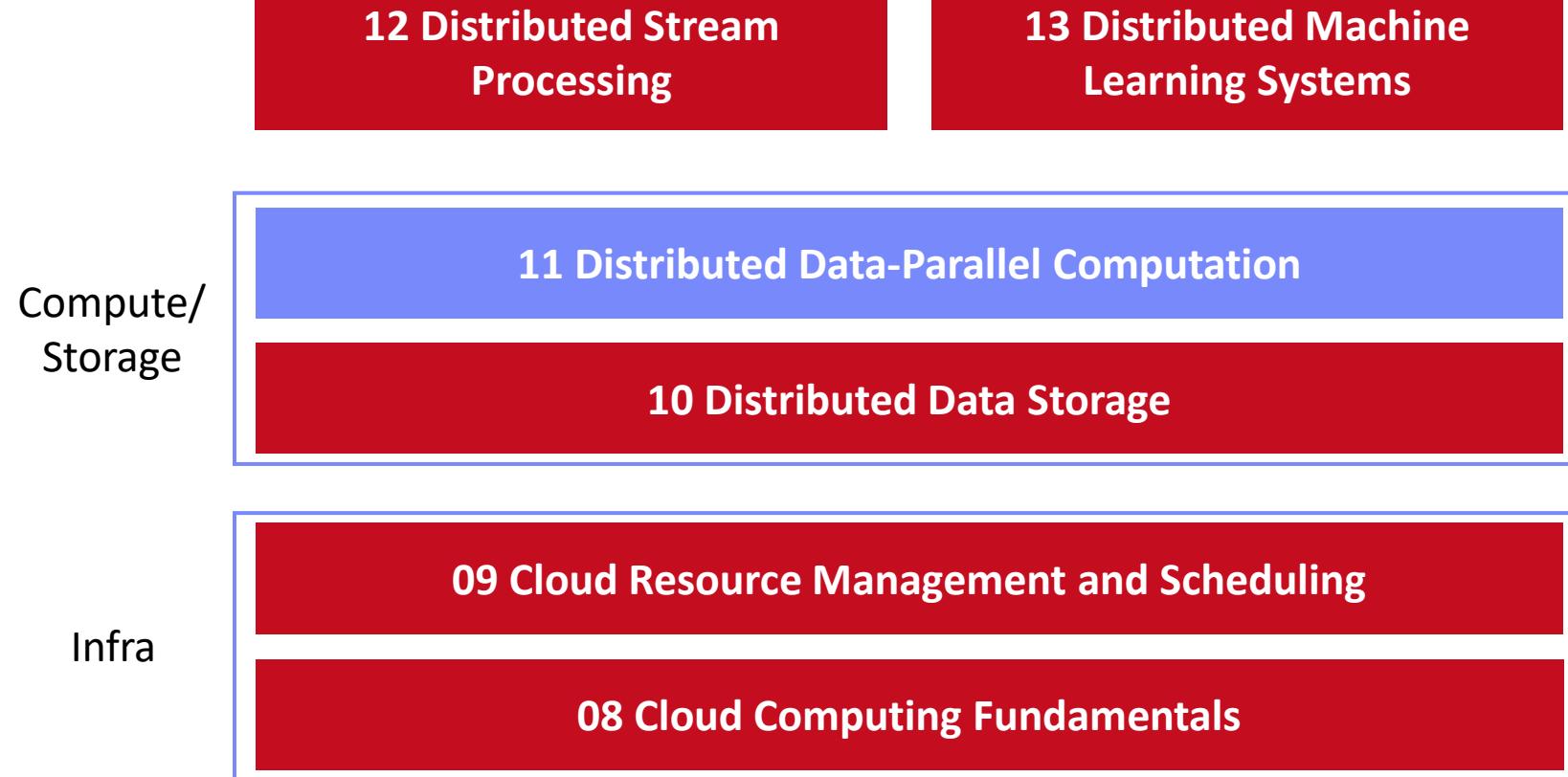
■ #1 Video Recording

- Hybrid lectures: in-person H 0107, zoom live streaming, video recording
- <https://tu-berlin.zoom.us/j/9529634787?pwd=R1ZsN1M3SC9BOU1OcFdmem9zT202UT09>

■ #2 Exam Registration

- Time slots: **Feb 08, 4pm or Feb 15, 4pm** (start 4.15pm, end 5.45pm, **48 seats per exam**)
- Sign up for exam via ISIS (once you submitted the project/exercise), **opens Jan 18**
- [If more capacity needed, additional slots Feb 08, 6pm and Feb 15, 6pm]

Course Outline Part B: Large-Scale Data Management and Analysis



Agenda



- Motivation and Terminology
- Data-Parallel Collection Processing
- Data-Parallel Data-Frame Operations
- Data-Parallel Computation in **SystemDS**

Motivation and Terminology

Recap: Central Data Abstractions



▪ #1 Files and Objects

- **File:** Arbitrarily large sequential data in specific file format (CSV, binary, etc)
- **Object:** binary large object, with certain meta data

▪ #2 Distributed Collections

- Logical multi-set (**bag**) of **key-value pairs** (**unsorted collection**)
- Different physical representations
- **Easy distribution** of pairs via horizontal partitioning (aka shards, partitions)
- Can be created from single file, or directory of files (unsorted)

Key	Value
4	Delta
2	Bravo
1	Alfa
3	Charlie
5	Echo
6	Foxtrot
7	Golf
1	Alfa

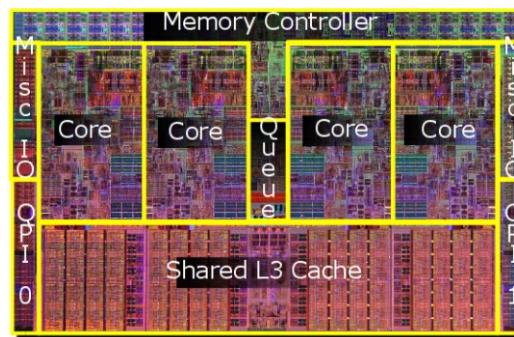
Excusus: Nehalem Architecture

[Michael E. Thomadakis: The Architecture of the Nehalem Processor and Nehalem-EP SMP Platforms, Report, 2010]



■ Multi-core CPU

- 4 core w/ hyper-threading
- **Per core:** L1i/L1d, L2 cache
- **Per CPU:** L3 cache (8MB)
- 3 memory channels
(8B width, max 1.333Ghz)



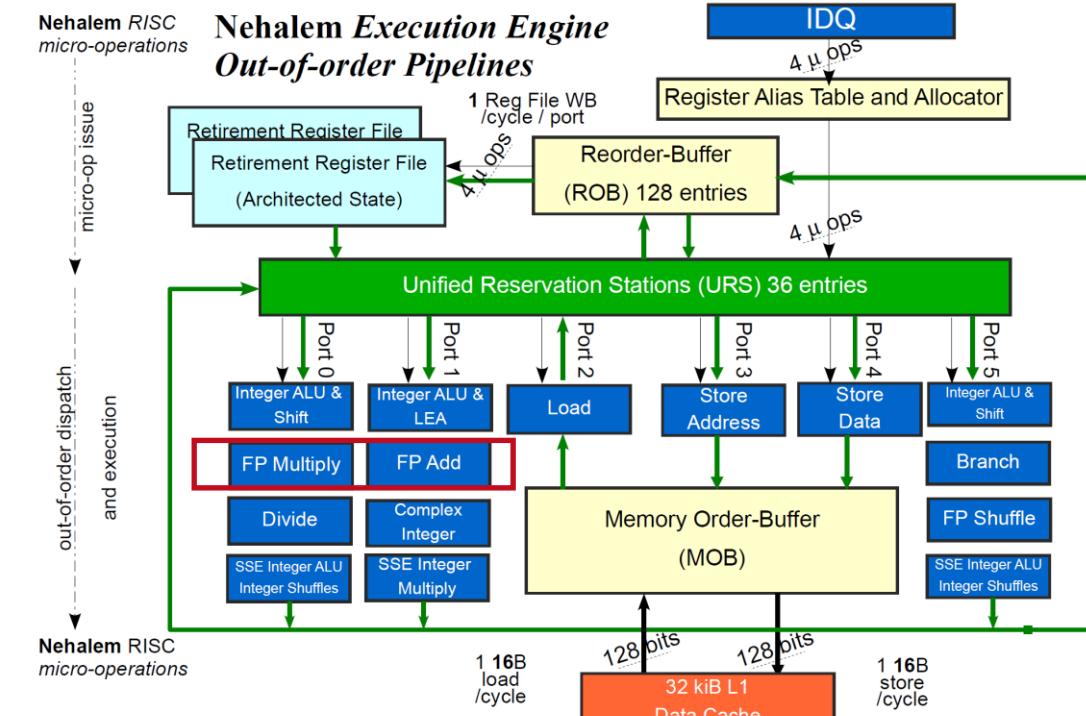
QPI ... Quick Path Interconnect

■ Instruction Pipeline

- **Frontend:** Instruction Fetch, Pre-Decode, and Decode
- **Backend:** Rename/Allocate, Scheduler, Execute, Write-Back

■ Out-of-Order Execution Engine (IPC=4)

- 128b FP Multiply
- 128b FP Add



Terminology Parallelism

▪ Flynn's Classification

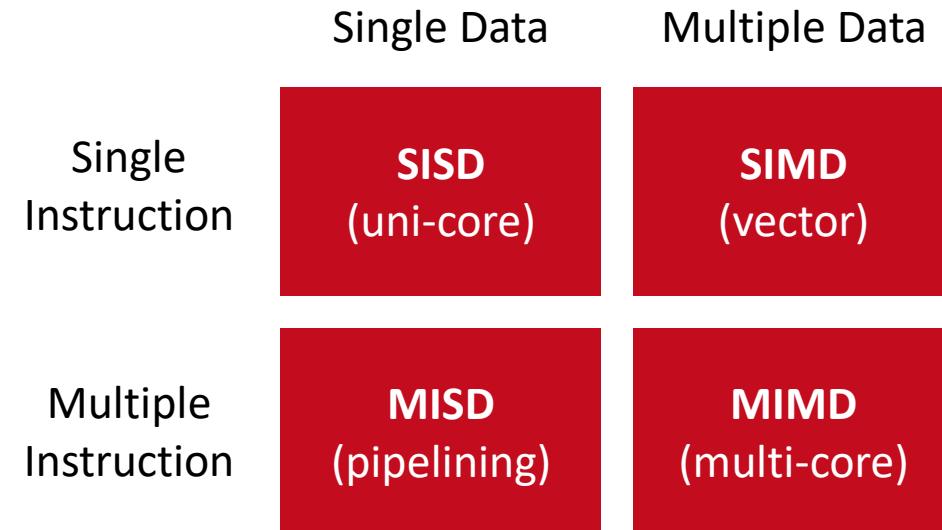
- SISD, SIMD
- (MISD), MIMD



[Michael J. Flynn, Kevin W. Rudd: Parallel Architectures. ACM Comput. Surv. 28(1) 1996]

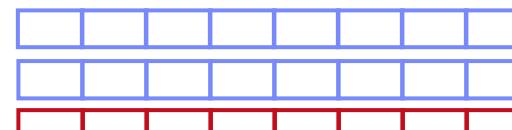
▪ Example: SIMD Processing

- Streaming SIMD Extensions (SSE)
- Process the same operation on multiple elements at a time (**packed** vs scalar SSE instructions)
- **Data parallelism** (aka: instruction-level parallelism)
- Example: **VFMADD132PD**



2009 Nehalem: **128b** (2xFP64)
 2012 Sandy Bridge: **256b** (4xFP64)
 2017 Skylake: **512b** (8xFP64)

```
c = _mm512_fmadd_pd(a, b);
a
b
c
```



Terminology Parallelism, cont.

▪ Distributed, Data-Parallel Computation

- Parallel computation of function `foo()` → **single instruction**
- Collection `X` of data items (key-value pairs) → **multiple data**
- Data parallelism similar to **SIMD** but more coarse-grained notion of “instruction” and “data”
→ **SPMD** (single program, multiple data)

$$Y = X.\text{map}(x \rightarrow \text{foo}(x))$$

[Frederica Darema: The SPMD Model : Past, Present and Future. **PVM/MPI 2001**]



▪ Additional Terminology

- **BSP**: Bulk Synchronous Parallel (global barriers)
- **ASP**: Asynchronous Parallel (no barriers, often with accuracy impact)
- **SSP**: Stale-synchronous parallel (staleness constraint on fastest-slowest)
- Other: Fork&Join, Hogwild!, event-based, decentralized

▪ Beware: **data parallelism** used in very different contexts (e.g., Parameter Server)

Data-Parallel Collection Processing

Hadoop History and Architecture

▪ Recap: Brief History

- Google's GFS [SOSP'03] + MapReduce
→ [Apache Hadoop](#) (2006)
- Apache Hive (SQL), Pig (ETL), Mahout/SystemML (ML), Giraph (Graph)

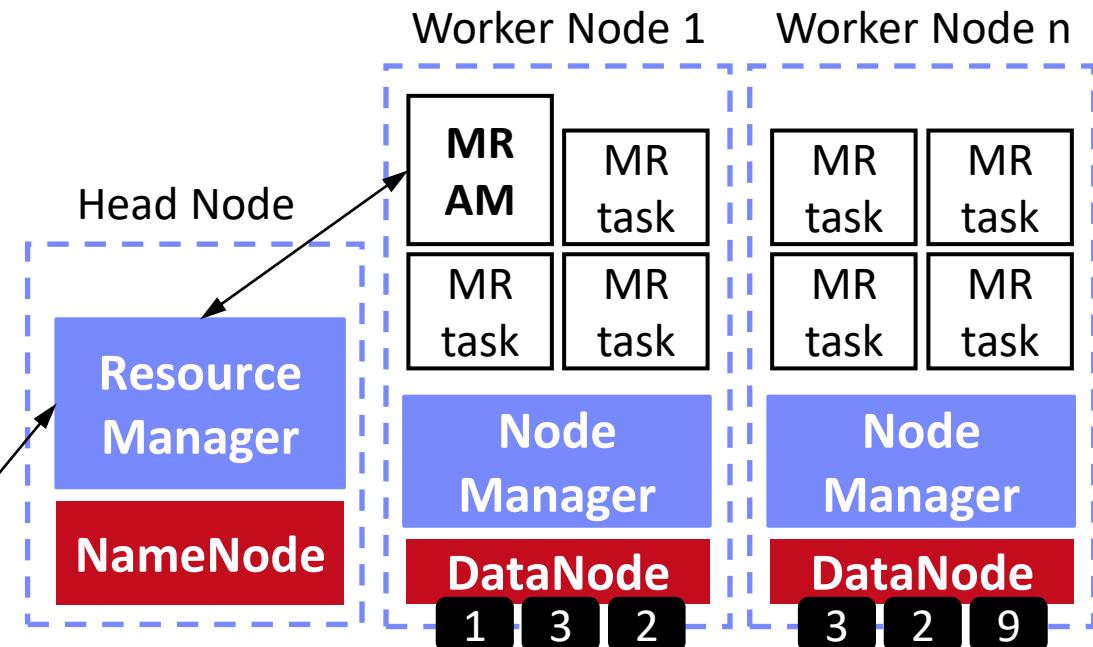


[Jeffrey Dean, Sanjay Ghemawat:
MapReduce: Simplified Data Processing
on Large Clusters. **OSDI 2004**]



▪ Hadoop Architecture / Eco System

- Management (Ambari)
- Coordination / workflows (Zookeeper, Oozie)
- Storage ([HDFS](#))
- Resources ([YARN](#))
[SoCC'13]
- Processing (**MapReduce**)



MapReduce – Programming Model



▪ Overview Programming Model

- Inspired by functional programming languages
- **Implicit parallelism** (abstracts distributed storage and processing)
- **Map** function: key/value pair → set of intermediate key/value pairs
- **Reduce** function: merge all intermediate values by key

▪ Example

```
SELECT Dep, count(*) FROM csv_files GROUP BY Dep
```

Name	Dep
X	CS
Y	CS
A	EE
Z	CS

Collection of
key/value pairs

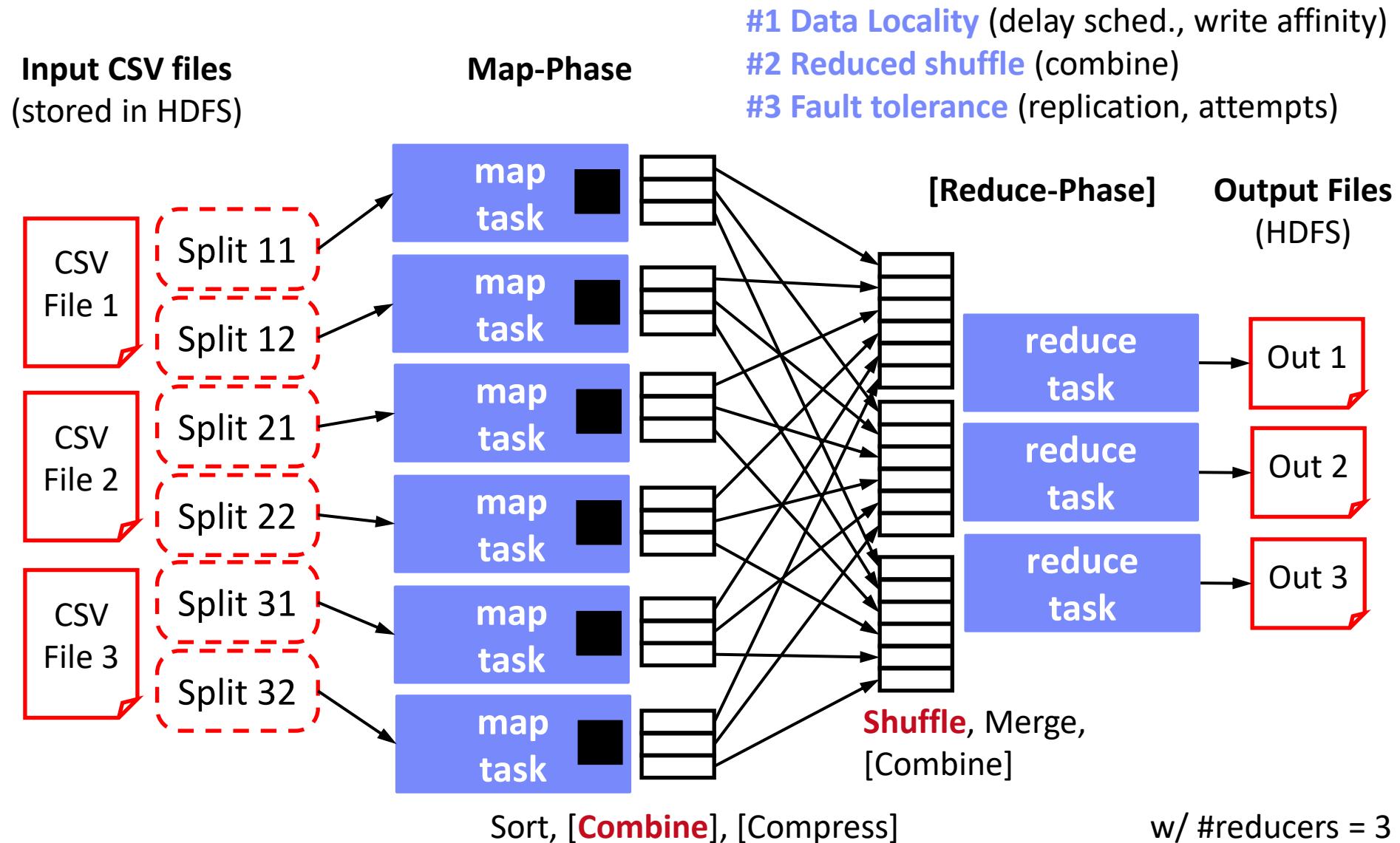
```
map(Long pos, String line) {  
    parts ← line.split(",")  
    emit(parts[1], 1)  
}
```

CS	1
CS	1
EE	1
CS	1

```
reduce(String dep,  
       Iterator<Long> iter) {  
    total ← iter.sum();  
    emit(dep, total)  
}
```

CS	3
EE	1

MapReduce – Execution Model



▪ Basic Unary Operations

- Selections (brute-force), projections
- Ordering (e.g., **TeraSort**): Sample, pick k quantiles; shuffle-based partition sort
- Additive and semi-additive aggregation with grouping, distinct

▪ Binary Operations

- Set operations (union, intersect, difference) and joins
- Different physical operators for $R \bowtie S$
 - **Broadcast join**: broadcast S , build HT S , map-side HJOIN
 - **Repartition join**: shuffle (repartition) R and S , reduce-side MJOIN
 - **Improved repartition join**: avoid buffering via key-tag sorting
 - **Directed join** (pre/co-partitioned): map-only, R input, S read side-ways

[Spyros Blanas et al.: A comparison of join algorithms for log processing in MapReduce. **SIGMOD 2010**]



▪ Hybrid SQL-on-Hadoop Systems

- E.g.: Hadapt (HadoopDB), Impala, IBM BigSQL, Presto, Drill, Actian

[Daniel Abadi, Shivnath Babu, Fatma Ozcan, Ippokratis Pandis: Tutorial: SQL-on-Hadoop Systems. **PVLDB 2015**]



▪ Summary MapReduce

- Large-scale & fault-tolerant processing w/ UDFs and files → **Flexibility**
- Restricted functional APIs → **Implicit parallelism and fault tolerance**
- **Criticism:** #1 **Performance**, #2 **Low-level APIs**, #3 **Many different systems**

▪ Evolution to Spark (and Flink)

- Spark [HotCloud'10] + RDDs [NSDI'12] → **Apache Spark** (2014)
- **Design:** **standing executors with in-memory storage**, lazy evaluation, fault-tolerance via RDD lineage
- **Performance:** In-memory storage and fast job scheduling (100ms vs 10s)
- **APIs:** Richer functional APIs and general computation DAGs,
high-level APIs (e.g., DataFrame/Dataset), unified platform



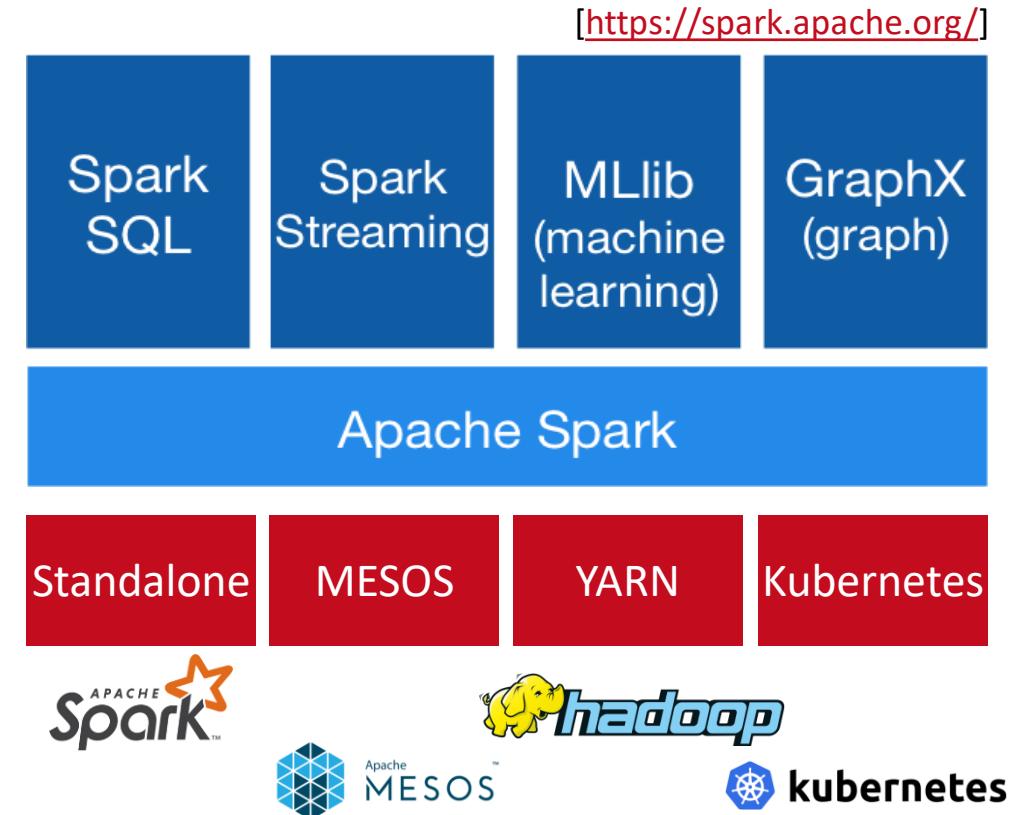
→ But many shared concepts/infrastructure

- **Implicit parallelism through dist. collections** (data access, fault tolerance)
- Resource negotiators (YARN, Mesos, Kubernetes)
- HDFS and object store connectors (e.g., Swift, S3)

Spark History and Architecture, cont.

▪ High-Level Architecture

- **Different language bindings:**
Scala, Java, Python, R
- **Different libraries:**
SQL, ML, Stream, Graph
- Spark core (incl RDDs)
- **Different cluster managers:**
Standalone, Mesos, **Yarn**, **Kubernetes**
- Different file systems/
formats, and data sources:
HDFS, **S3**, **SWIFT**, **DBs**, **NoSQL**



- Focus on a **unified platform**
for data-parallel computation (**Apache Flink** w/ similar goals)

Spark Resilient Distributed Datasets (RDDs)



■ RDD Abstraction

- **Immutable**, partitioned collections of key-value pairs
- **Coarse-grained** deterministic operations (transformations/actions)
- Fault tolerance via lineage-based re-computation

`JavaPairRDD<MatrixIndexes, MatrixBlock>`

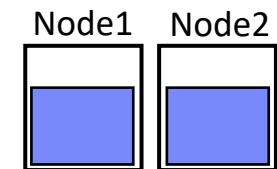
■ Operations

- **Transformations**: define new RDDs
- **Actions**: return result to driver

■ Distributed Caching

- Use fraction of worker **memory for caching**
- Eviction at granularity of individual partitions
- **Different storage levels** (e.g., mem/disk x serialization x compression)

Type	Examples
Transformation (lazy)	<code>map</code> , <code>hadoopFile</code> , <code>textFile</code> , <code>flatMap</code> , <code>filter</code> , <code>sample</code> , <code>join</code> , <code>groupByKey</code> , <code>cogroup</code> , <code>reduceByKey</code> , <code>cross</code> , <code>sortByKey</code> , <code>mapValues</code>
Action	<code>reduce</code> , <code>save</code> , <code>collect</code> , <code>count</code> , <code>lookupKey</code>

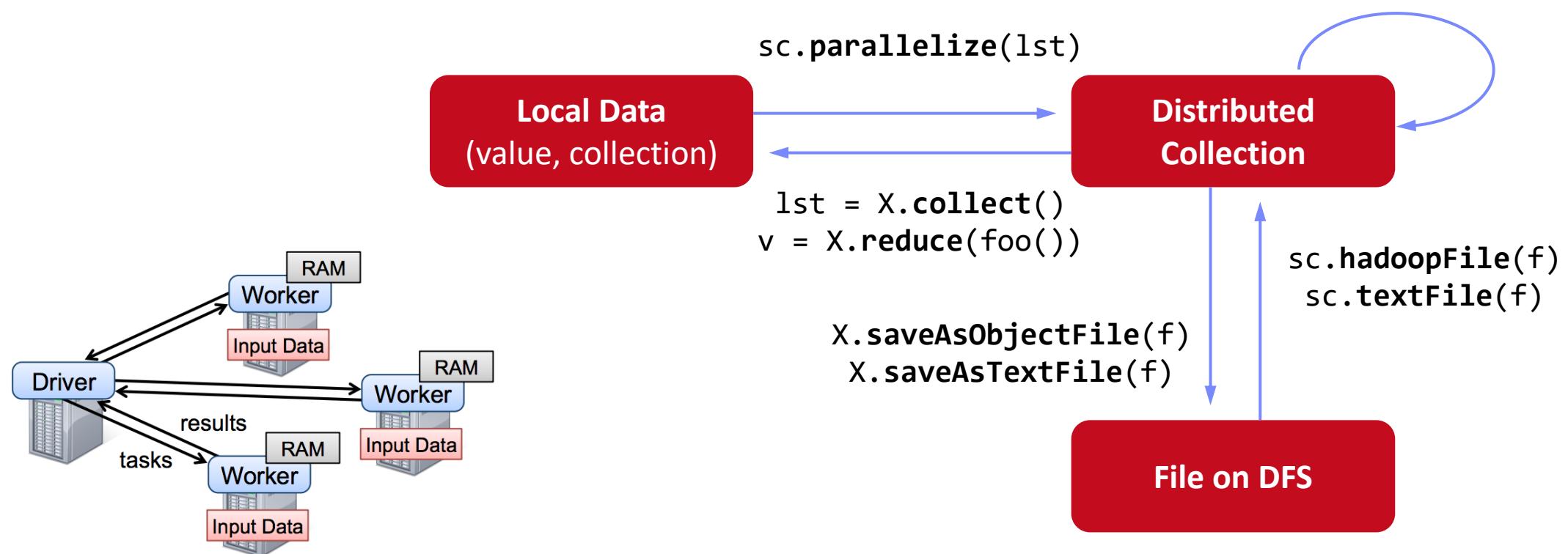


Spark Resilient Distributed Datasets (RDDs), cont.



Lifecycle of an RDD

- Note: can't broadcast an RDD directly



Spark Partitions and Implicit/Explicit Partitioning

■ Spark Partitions

- Logical key-value collections are split into **physical partitions**
- Partitions are granularity of **tasks, I/O, shuffling, evictions**

~128MB

■ Partitioning via Partitioners

- Implicitly on every data shuffling
- Explicitly via `R.repartition(n)`

Example Hash Partitioning:

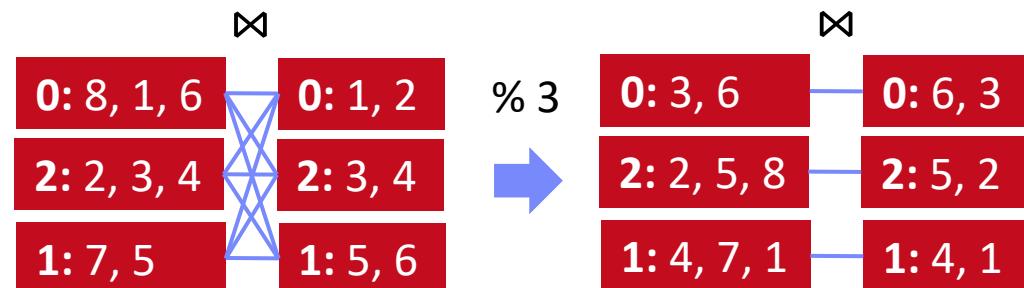
For all (k, v) of R :
 $pid = \text{hash}(k) \% n$

■ Partitioning-Preserving

- All operations that are guaranteed to keep keys unchanged
(e.g. `mapValues()`, `mapPartitions()` w/ `preservesPart` flag)

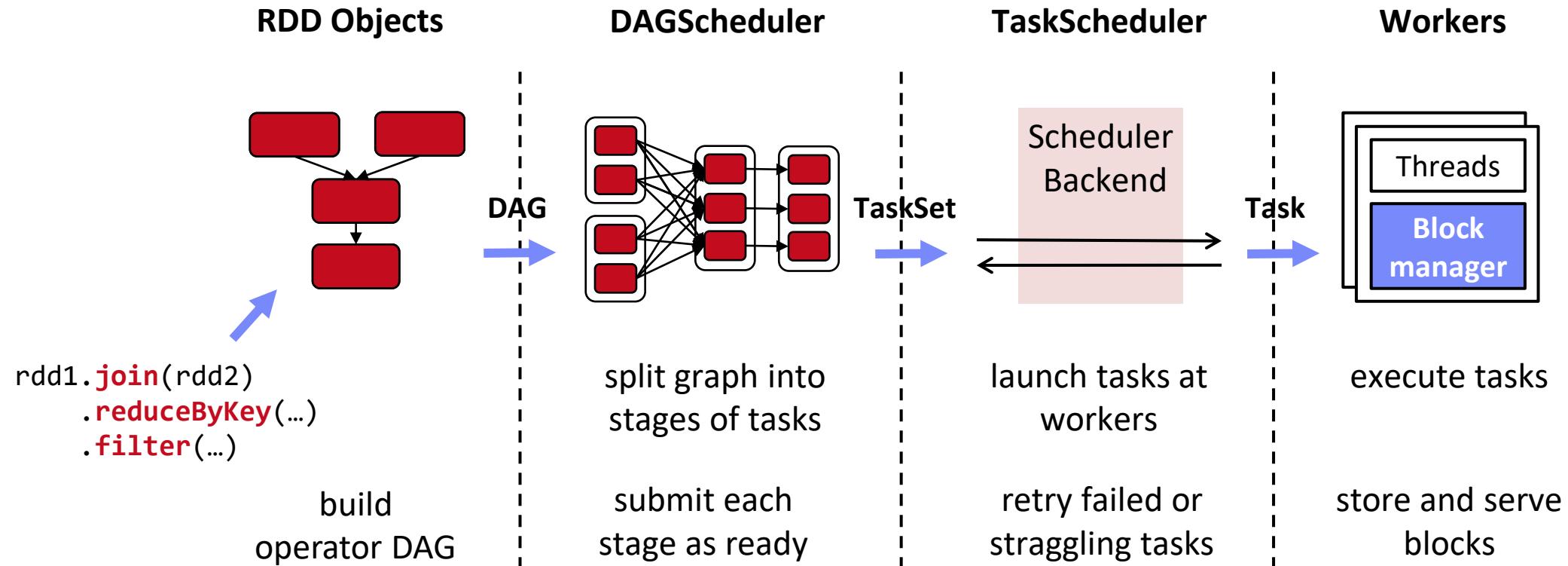
■ Partitioning-Exploiting

- Join: $R3 = R1.join(R2)$
- Lookups:
 $v = C.lookup(k)$

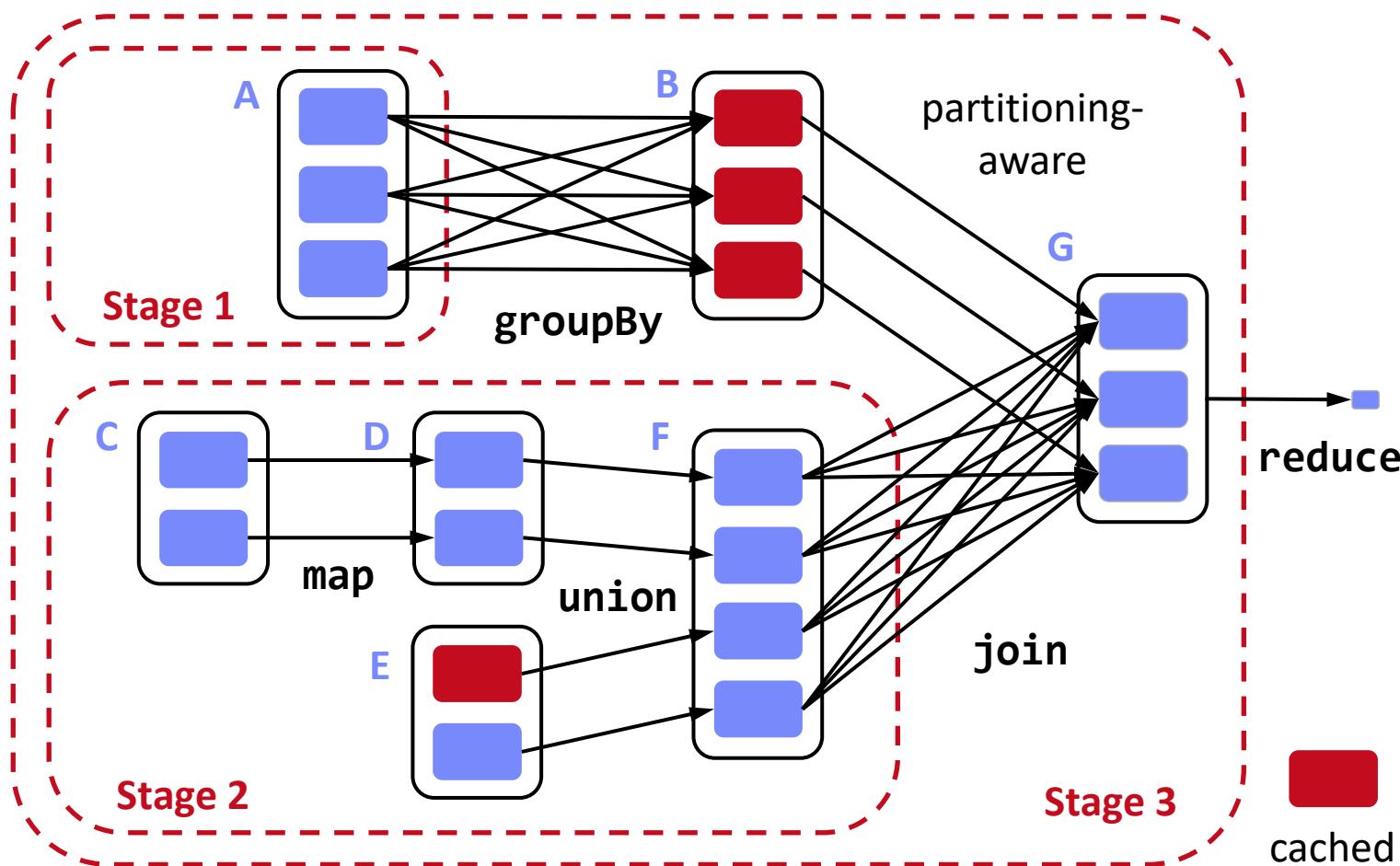


Spark Scheduling Process

[Tilmann Rabl:
Big Data Systems,
HPI WS2019/20]



Spark Lazy Evaluation, Caching, and Lineage



[Matei Zaharia, Mosharaf Chowdhury, Tathagata Das, Ankur Dave, Justin Ma, Murphy McCauly, Michael J. Franklin, Scott Shenker, Ion Stoica: Resilient Distributed Datasets: A Fault-Tolerant Abstraction for In-Memory Cluster Computing. NSDI 2012]



1. Reduce action triggers DAG compilation and evaluation
2. DAG compiled into job of multiple stages (3 here), demarcated by wide shuffle dependencies
3. Lost/evicted cached partitions are re-evaluated via partition lineage

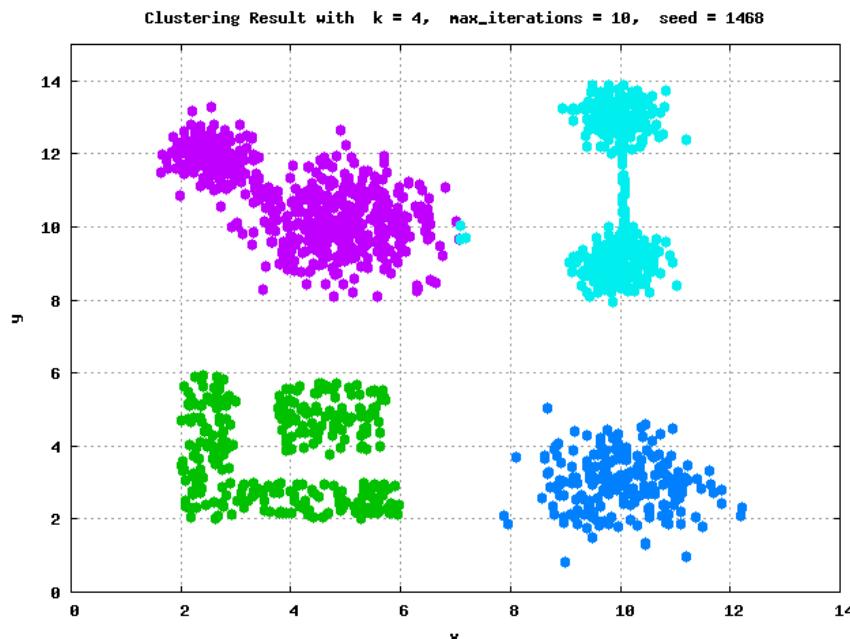
Example: k-Means Clustering

■ k-Means Algorithm

- Given dataset D and number of clusters k, find cluster centroids (“mean” of assigned points) that minimize within-cluster variance
- Euclidean distance: $\sqrt{\sum((a-b)^2)}$

■ Pseudo Code

```
function Kmeans(D, k, maxiter) {
    C' = randCentroids(D, k);
    C = {};
    i = 0; //until convergence
    while( C' != C & i<=maxiter ) {
        C = C';
        i = i + 1;
        A = getAssignments(D, C);
        C' = getCentroids(D, A, k);
    }
    return C'
}
```



Example: k-Means Clustering in Spark



```
// create spark context (allocate configured executors)
JavaSparkContext sc = new JavaSparkContext();

// read and cache data, initialize centroids
JavaRDD<Row> D = sc.textFile("hdfs:/user/mboehm/data/D.csv")
    .map(new ParseRow()).cache(); // cache data in spark executors
Map<Integer,Mean> C = asCentroidMap(D.takeSample(false, k));

// until convergence
while( !equals(C, C2) & i<=maxiter ) {
    C2 = C; i++;
    // assign points to closest centroid, recompute centroid
    Broadcast<Map<Integer,Row>> bC = sc.broadcast(C)
    C = D.mapToPair(new NearestAssignment(bC))
        .foldByKey(new Mean(0), new IncComputeCentroids())
        .collectAsMap();
}
return C;
```

Note: Existing library algorithm

[<https://github.com/apache/spark/blob/master/mllib/src/main/scala/org/apache/spark/mllib/clustering/KMeans.scala>]

Data-Parallel Data-Frame Operations

■ Recap: Data Preparation Problem

- **80% Argument:** 80-90% time for finding, integrating, cleaning data
- Data scientists prefer scripting languages and in-memory libraries



■ R and Python DataFrames

- R `data.frame/dplyr` and Python `pandas DataFrame` for seamless data manipulations (most popular packages/features)
- DataFrame: **table with a schema**
- Descriptive stats and basic math, reorganization, joins, grouping, windowing
- **Limitation:** Only in-memory, single-node operations

■ Example

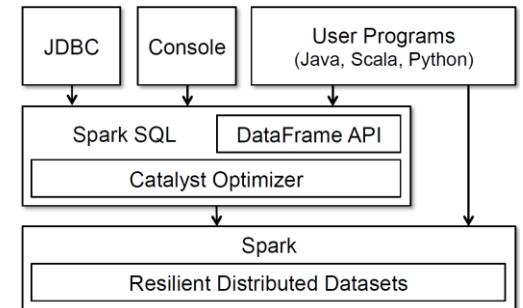
```
import pandas as pd  
Pandas      df = pd.read_csv('data/tmp1.csv', index_col=2)  
              df.head() # df w/ indexes A-Z  
  
              df = pd.concat(df, df[['A','C']], axis=0)
```

Spark DataFrames and DataSets



■ Overview Spark DataFrame

- DataFrame is a **distributed collection of rows** with named/typed columns
- **Relational operations** (e.g., projection, selection, joins, grouping, aggregation)
- **DataSources** (e.g., json, jdbc, parquet, hdfs, s3, avro, hbase, csv, cassandra)



■ DataFrame and Dataset APIs

- DataFrame was introduced as basis for Spark SQL
- DataSets allow **more customization** and compile-time analysis errors (Spark 2)

DataFrame = Dataset[Row]

■ Example DataFrame

```
logs = spark.read.format("json").open("s3://logs")
logs.groupBy(logs.user_id).agg(sum(logs.time))
    .write.format("jdbc").save("jdbc:mysql//...")
```



[Michael Armbrust: Structuring Apache Spark – SQL, DataFrames, Datasets, and Streaming, **Spark Summit 2016**]

→ PySpark

SparkSQL and DataFrame/Dataset



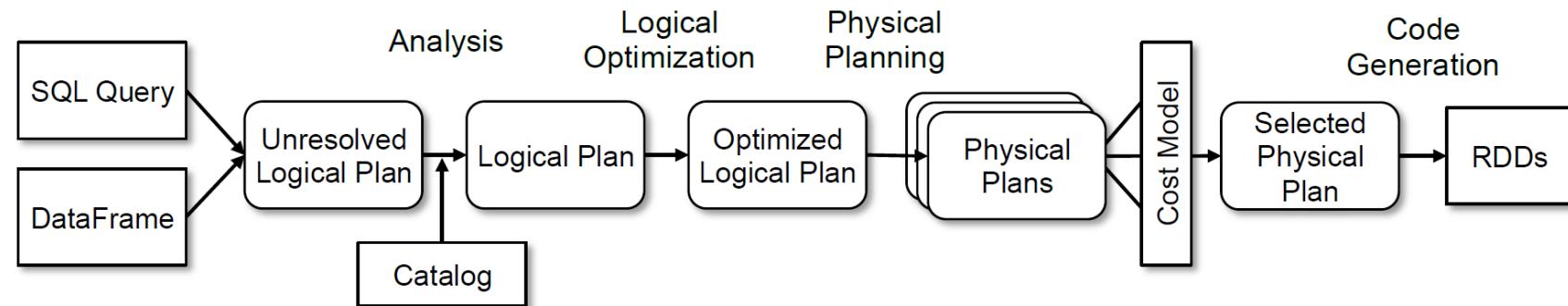
▪ Overview SparkSQL

- Shark (~2013): academic prototype for SQL on Spark
- **SparkSQL** (~2015): reimplemented from scratch
- Common IR and compilation of SQL and DataFrame operations

[Michael Armbrust et al.: Spark SQL: Relational Data Processing in Spark. **SIGMOD 2015**]



▪ Catalyst: Query Planning



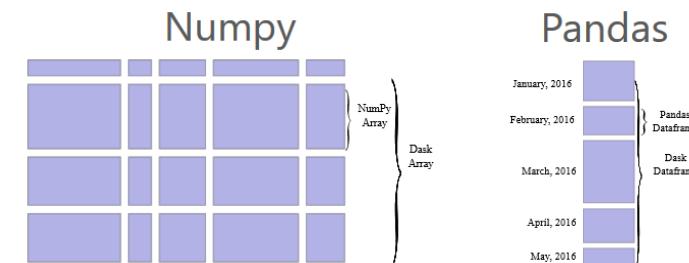
▪ Performance features

- #1 **Whole-stage code generation** via Janino
- #2 **Off-heap memory** (`sun.misc.Unsafe`) for caching and certain operations
- #3 **Pushdown** of selection, projection, joins into data sources (+ join ordering)



■ Overview Dask

- Multi-threaded and distributed operations for arrays, bags, and dataframes
- **dask.array**: list of numpy n-dim arrays
- **dask.dataframe**: list of pandas data frames
- **dask.bag**: unordered list of tuples (second order functions)
- **Local and distributed schedulers**:
threads, processes, YARN, Kubernetes, containers, HPC, and cloud, GPUs



■ Execution

- **Lazy evaluation**
- Limitation: requires **static size inference**
- Triggered via `compute()`

■ Discussion

- PySpark Competition (but not out-of-core), scalable ML algorithms via <https://ml.dask.org/> (partnering w/ scikit-learn)

```
import dask.array as da
x = da.random.random(
    (10000,10000), chunks=(1000,1000))
y = x + x.T
y.persist() # cache in memory
z = y[::2, 5000:].mean(axis=1) # colMeans
ret = z.compute() # returns NumPy array
```

Modin (UC Berkeley → Ponder → Snowflake)

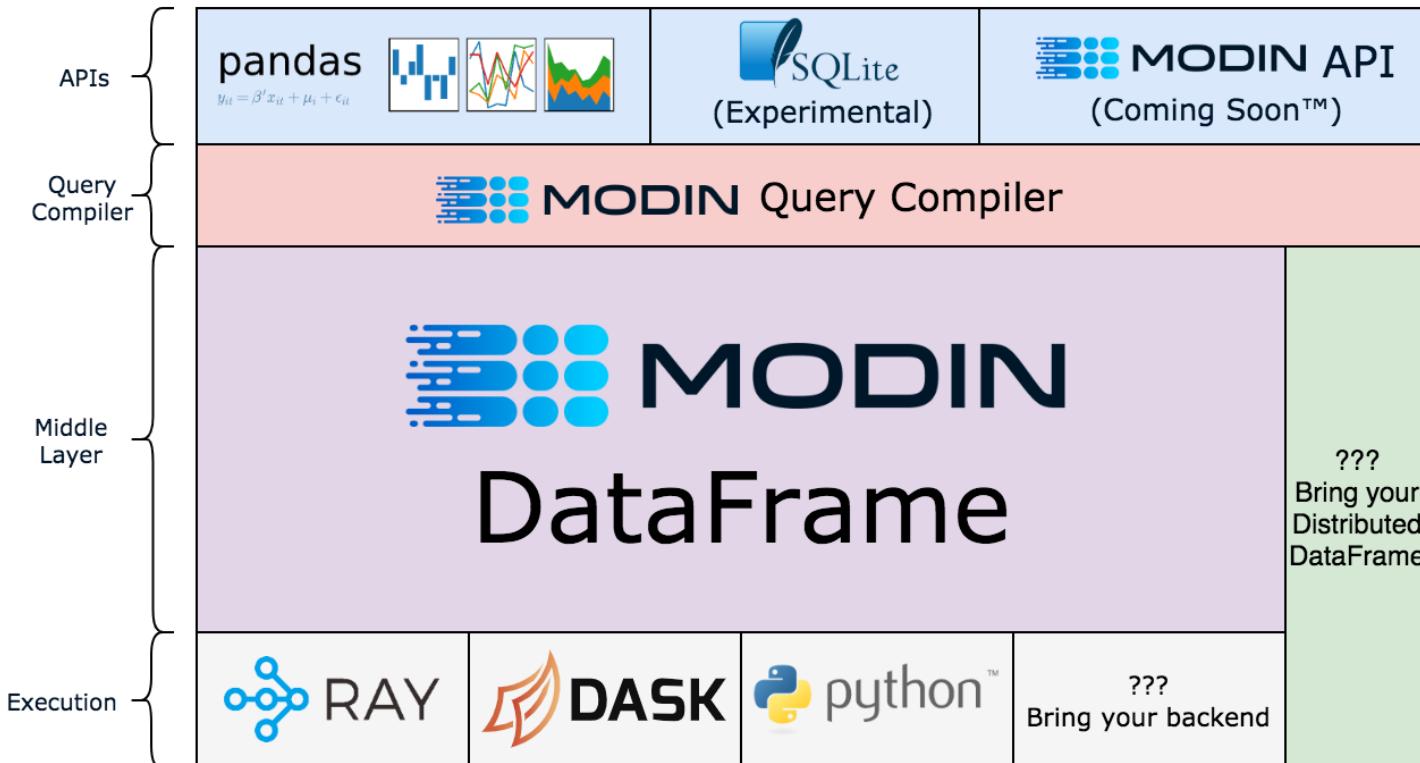
[Devin Petersohn, et al.:
Towards Scalable Dataframe
Systems. **PVLDB 2020**]



▪ Overview Modin

- Goal: Enhance **Pandas data frames**
- Convert Pandas API to **core algebra expressions**
- Different Backends:
Ray, Dask, MPI

[\[https://github.com/
modin-project/modin\]](https://github.com/modin-project/modin)



Data-Parallel Computation in SystemDS



[Matthias Boehm et al.: SystemDS: A Declarative Machine Learning System for the End-to-End Data Science Lifecycle. **CIDR 2020**]

[Matthias Boehm et al.: SystemML: Declarative Machine Learning on Spark. **PVLDB 2016**]

[Amol Ghoting et al.: SystemML: Declarative Machine Learning on MapReduce. **ICDE 2011**]

Background: Matrix Formats



■ Matrix Block ($m \times n$)

- A.k.a. tiles/chunks, most operations defined here
- Local matrix: single block, different representations

■ Common Block Representations

- Dense (linearized arrays)
- MCSR (modified CSR)
- CSR (compressed sparse rows), CSC
- DCSR (double compressed sparse rows)
- COO (Coordinate matrix)

Dense (row-major)

.7	0	.1	.2	.4	0	0	.3	0
----	---	----	----	----	---	---	----	---

$O(mn)$

Example
3x3 Matrix

.7		.1
.2	.4	
	.3	

DIA23/24 project
(Jannik Lindemann):
DCSR



MCSR

0	2	
.7	.1	
0	1	
.2	.4	
1		
.3		

$O(m + nnz(X))$

CSR

0	0	.7
2	2	.1
4	0	.2
5	1	.4
1	1	.3

$O(nnz(X))$

COO

0	0	.7
0	2	.1
1	0	.2
1	1	.4
2	1	.3

Distributed Matrix Representations



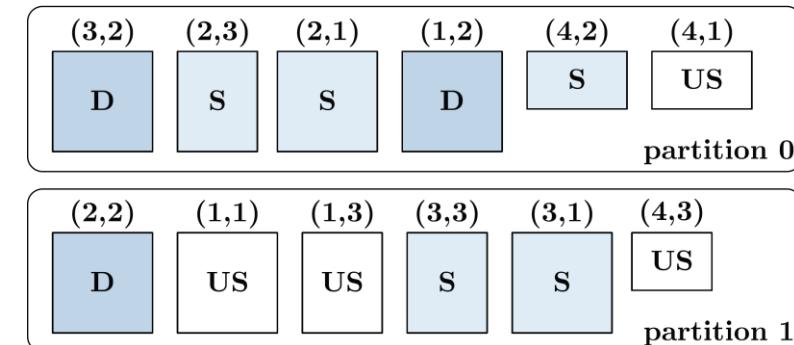
- Collection of “Matrix Blocks” (and keys)
 - Bag semantics (duplicates, unordered)
 - Logical (Fixed-Size) Blocking
 - + join processing / independence
 - (sparsity skew)
 - E.g., SystemML on Spark:
`JavaPairRDD<MatrixIndexes,MatrixBlock>`
 - Blocks encoded independently (dense/sparse)

- Partitioning
 - Logical Partitioning
(e.g., row-/column-wise)
 - Physical Partitioning
(e.g., hash / grid)
 - Influences partition-local aggregation

Logical Blocking
3,400x2,700 Matrix
(w/ $B_c=1,000$)

(1,1)	(1,2)	(1,3)
(2,1)	(2,2)	(2,3)
(3,1)	(3,2)	(3,3)
(4,1)	(4,2)	(4,3)

hash partitioned: e.g., $\text{hash}(3,2) \rightarrow 99.994 \% 2 = 0$



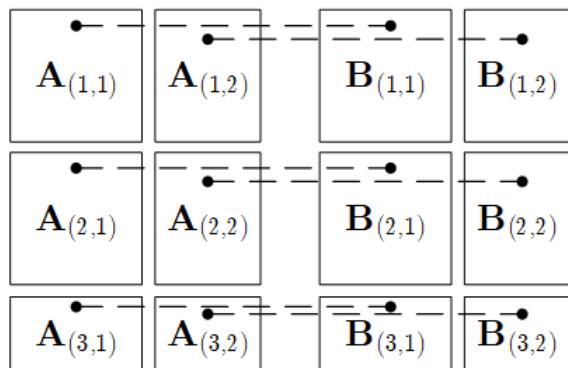
Distributed Matrix Operations

Q: How to implement these operations
with Spark RDD Operations?



Elementwise Multiplication (Hadamard Product)

$$C = A * B$$

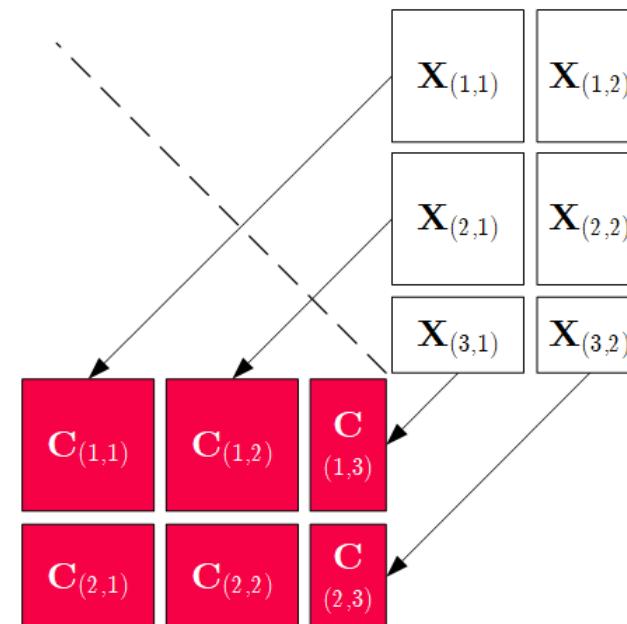


1:1 join

Note: also with
row/column vector rhs

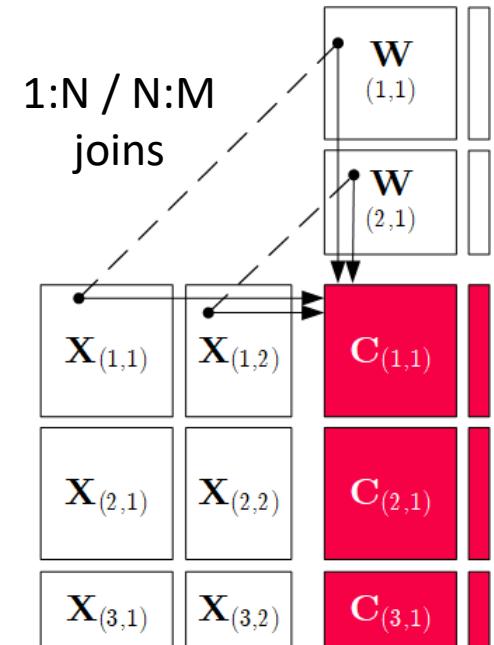
Transposition

$$C = t(X)$$



Matrix Multiplication

$$C = X \%*\% W$$



Partitioning-Preserving Operations



- **Shuffle is major bottleneck for ML on Spark**
- **Preserve Partitioning**
 - Op is partitioning-preserving if keys unchanged (guaranteed)
 - Implicit: Use restrictive APIs (`mapValues()` vs `mapToPair()`)
 - Explicit: Partition computation w/ declaration of partitioning-preserving

- **Exploit Partitioning**
 - Implicit: Operations based on `join`, `cogroup`, etc
 - Explicit: Custom operators (e.g., `zipmm`)

- **Example: Multiclass SVM**
 - Vectors fit neither into driver nor broadcast
 - $\text{ncol}(X) \leq B_c$

```
parfor(iter_class in 1:num_classes) {  
    Y_local = 2 * (Y == iter_class) - 1  
    g_old = t(X) %*% Y_local  
    ...  
    while( continue ) {  
        Xd = X %*% s  
        ... inner while loop (compute step_sz)  
        Xw = Xw + step_sz * Xd;  
        out = 1 - Y_local * Xw;  
        out = (out > 0) * out;  
        g_new = t(X) %*% (out * Y_local) ...  
    }  
}
```

Annotations:

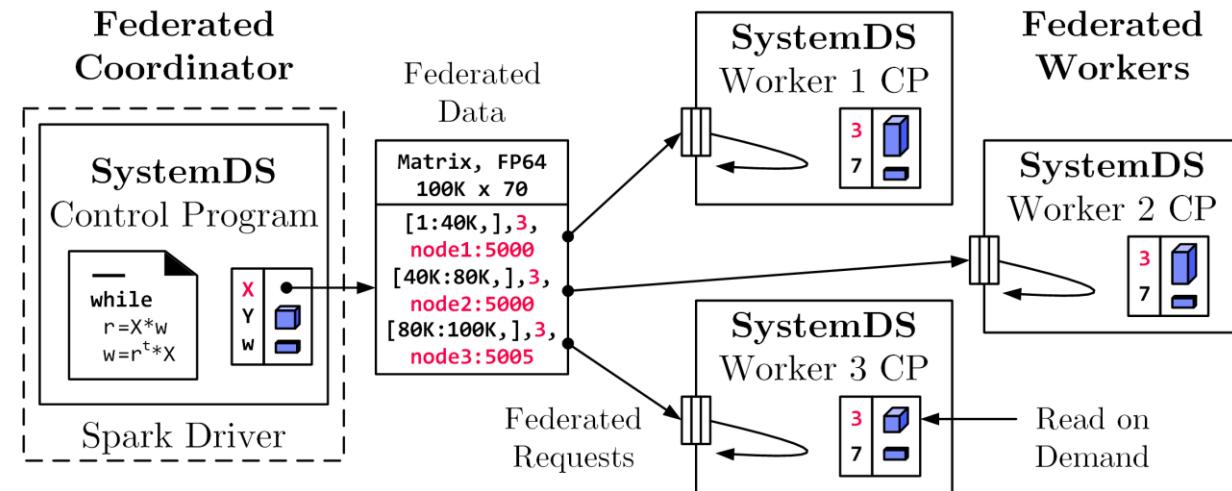
- parfor, chkpt X MEM_DISK
- chkpt y_local MEM_DISK
- chkpt Xd, Xw MEM_DISK
- zipmm

Federated Matrices / Frames

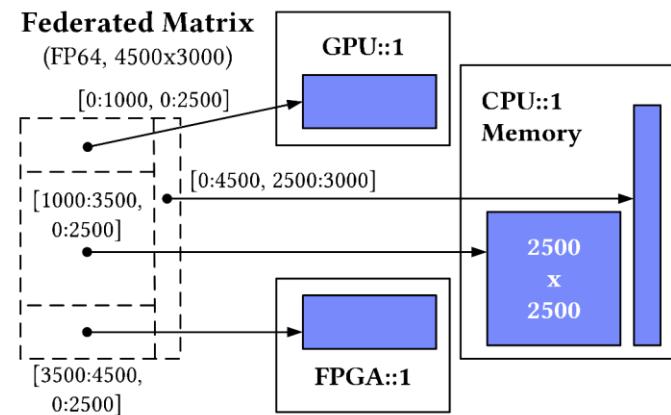


■ Federated Matrices

- Metadata on coordinator
- Disjoint tiles at federated sites
- Data-parallel operations on federated data



■ Generalization to Multi-device Settings



- Motivation and Terminology
- Data-Parallel Collection Processing
- Data-Parallel Data-Frame Operations
- Data-Parallel Computation in **SystemDS**

- Next Lectures (**Large-scale Data Management and Analysis**)
 - 12 [Distributed Stream Processing](#) [Jan 25]
 - 13 [Distributed Machine Learning Systems](#) [Feb 01]