Bringing the HPC Reconstruction Algorithms to Big Data Platforms

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New York Scientific Data Summit:
Data-Driven Discovery

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BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

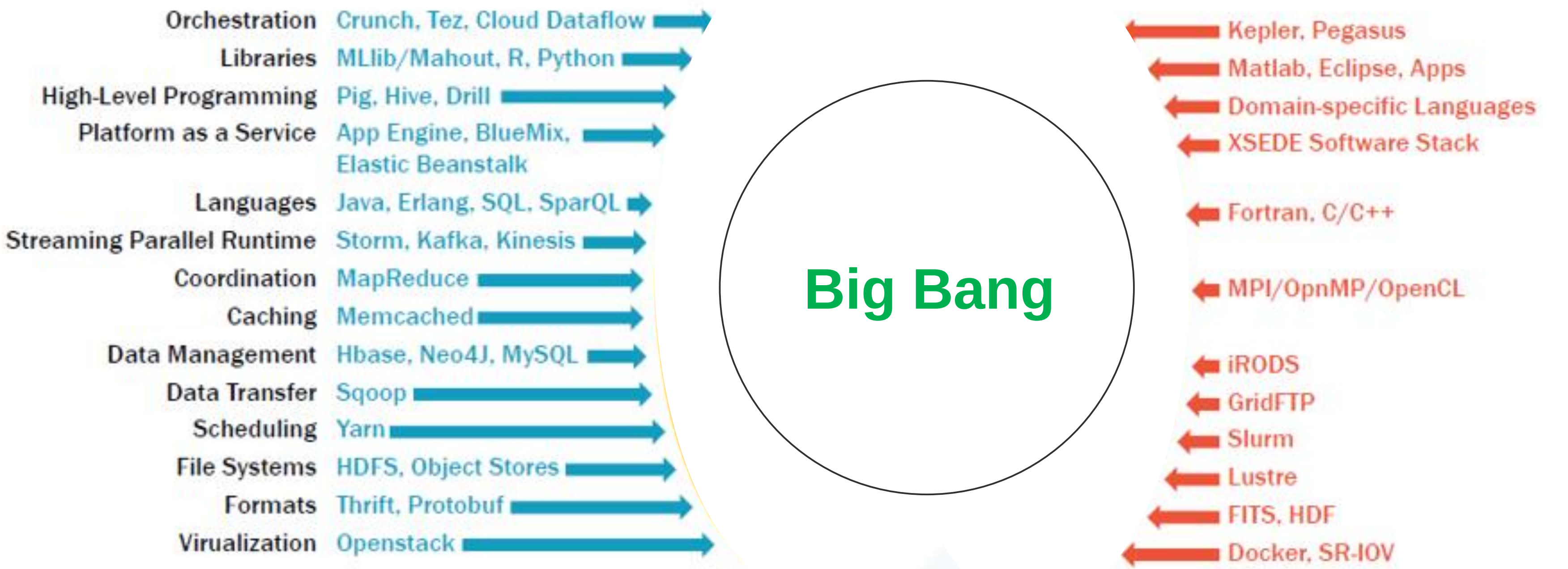
U.S. DEPARTMENT OF ENERGY | Office of Science

Outline

- Spark as an integrated platform for the Big Data and Big Computing applications
- Spark In-Situ Data Access Approach
- Ptychographic Application
- Spark-Based Distributed Deep Learning Solvers
- SHARP-SPARK Project
- Summary

Closing a Gap between Big Data and Big Computing

Ecosystems*: **Big Data** **Big Computing**



Motivation: **New Frontiers**

Leaders: **Spark** **MPI**

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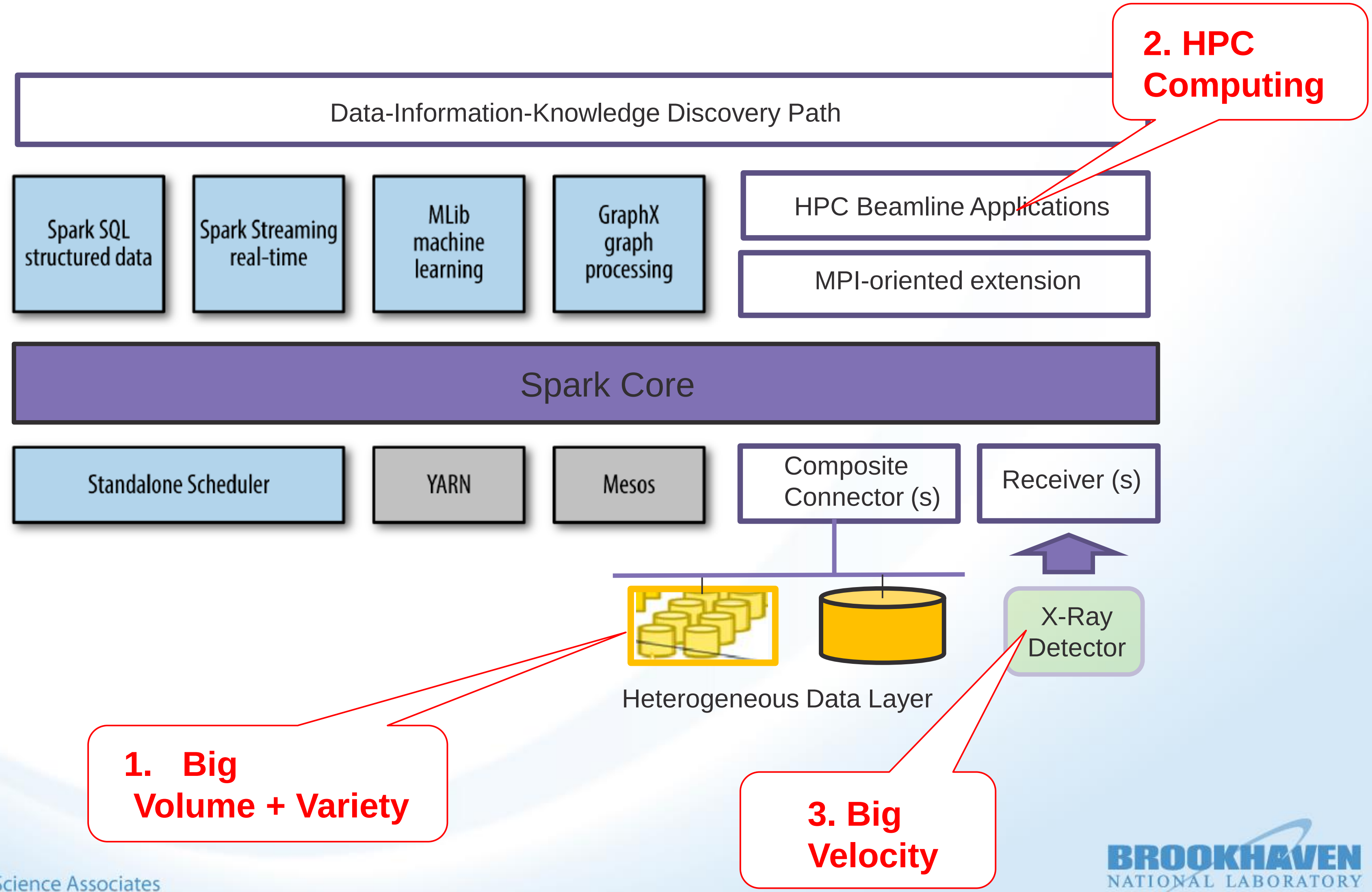
*G. Fox at al. HPC-ABDC High Performance Computing Enhanced Apache Big Data Stack, CCGrid, 2015

Three Directions

- ❑ Spark Model + MPI-oriented extension
- ❑ MPI Model + Spark-oriented extension
- ❑ New Model

topic of this talk

Spark ecosystem and proposed extensions for experimental facilities



DATA LAYER

Database vs HDF5 models

No SQL

RDB

Array-Oriented Model:
- *SciDB, MonetDB, etc.*

Column Family Model:
- *Bigtable, Cassandra, etc.*

Document-Oriented Model:
- *MongoDB, CouchDB, etc.*

Graph Model:
- *Neo4j, etc.*

HDF5

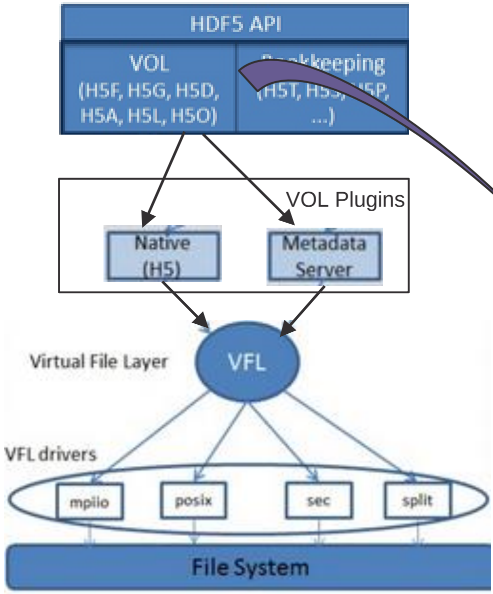
The HDF Group

The key data model concepts:

- **Group** - a collection of objects (including groups)
- **Dataset** - a multidimensional array of data elements with attributes and other metadata
- **Datatype** - a description of a specific class of data element
- **Attribute** - a named data value associated with a group, dataset, or named datatype

Present version: single file oriented

Large-Scale HDF5-Oriented Development

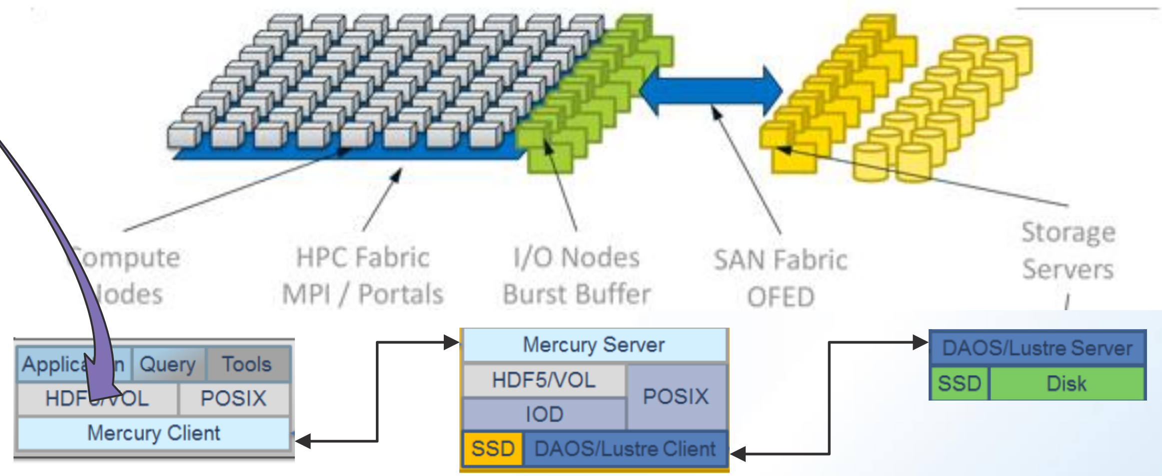


HDF5 Virtual Object Layer

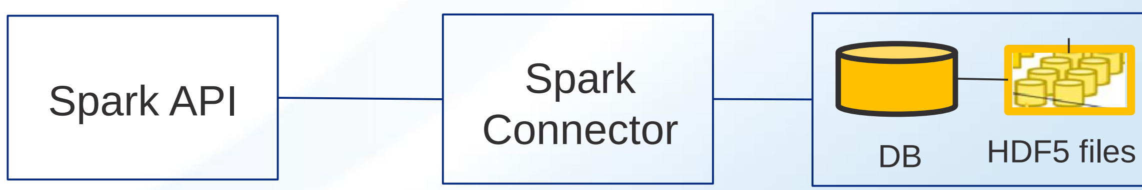
Exascale Fast-Forward I/0 and Storage Stack*

Time: 2012-2014

Team: Intel, The HDF Group, EMC, Cray

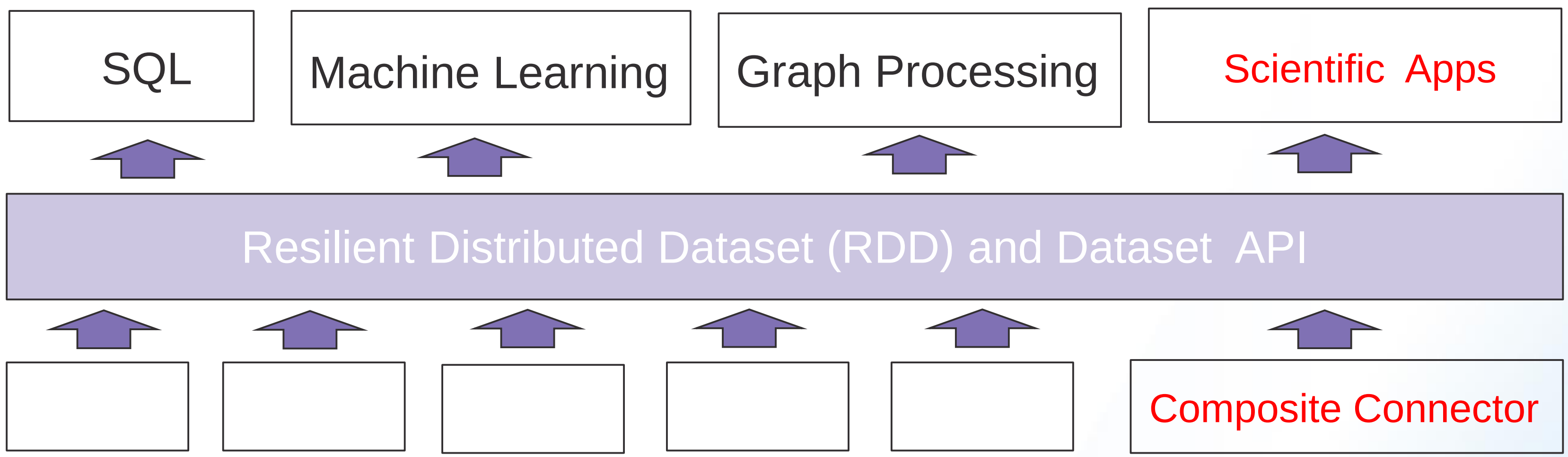


Spark-based Proposal



Intel, The HDF Group, EMC, and Cray. FF-Storage Final Report, June 2014

Spark In-Situ Data Access Approach

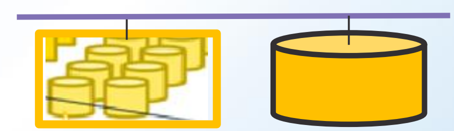


Supported file formats:

- Text files (plain, JSON, CSV)
- Hadoop InputFormat with arbitrary key and value
- Hadoop SequenceFile with arbitrary key and value
- Object files with the RDD values previously saved using the Java/Python serialization
- HDF5 (research projects*)

SQL and NoSQL Databases:

- Java Database Connectivity (JDBC)
- HBase
- Cassandra
- MongoDB
- Neo4j



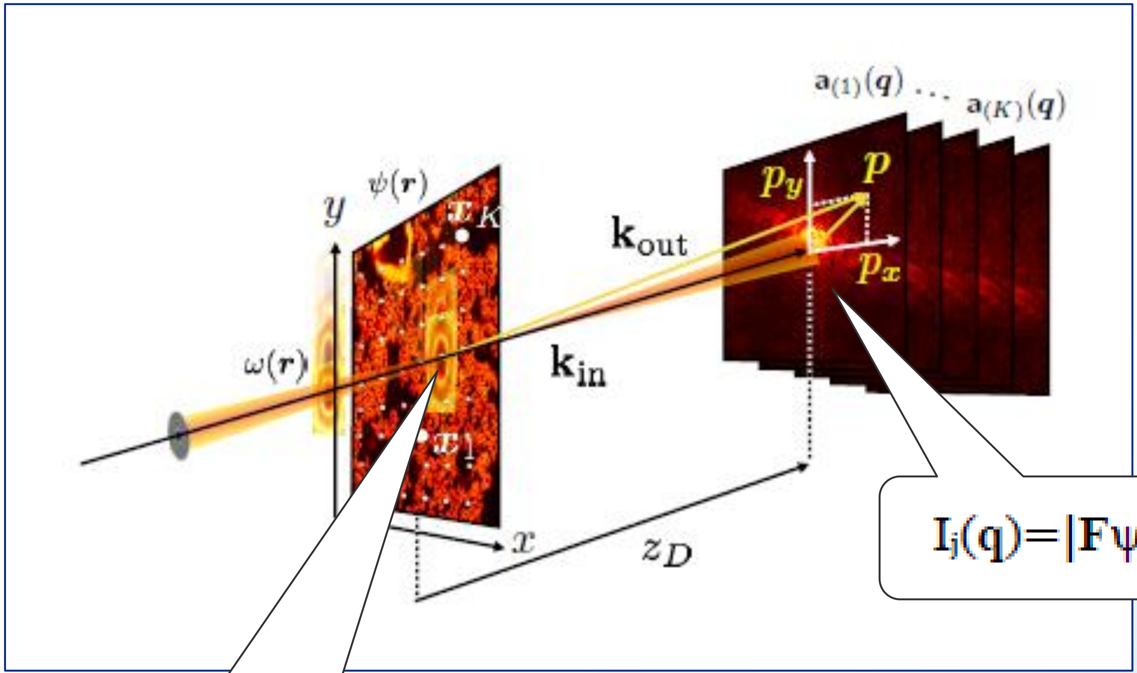
Heterogeneous Data Layer

J. Liu et al. H5Spark: Bridging the I/O Gap between Spark and Scientific Data Formats on HPC Systems, CUG, 2016

PTYCHOGRAPHIC APPLICATION

Ptychography

Ptychography is one of the essential image reconstruction techniques used in light source facilities. This method consists of measuring multiple diffraction patterns by scanning a finite illumination (also called the probe) on an extended specimen (the object).



$$I_j(q) = |F\psi_j|^2$$

$$\psi_j = P(r - r_j)O(r)$$

S. Marchesini et al. SHARP: a distributed, GPU-based ptychographiv solver, LBNL-1003977, January, 2016

Ptychography Algorithm (in math)

Iteration loop based on the difference map[1]:

$$\psi^{n+1} = \psi^{n} + \beta\,\Delta(\psi^{n})$$

$$\Delta = \pi_1 \circ f_2 - \pi_2 \circ f_1$$

$$f_i(\psi) = (1 + \gamma_i)\pi_i(\psi) - \gamma_i \psi$$

Projection operators associated with the modulus and overlap constraints:

$$\pi_a(\psi): \psi \rightarrow \mathbf{F}^* \frac{\mathbf{F}\psi}{|\mathbf{F}\psi|}\sqrt{I}$$

$$\pi_o(\psi): \psi \rightarrow P(\mathbf{r}-\mathbf{r}_j)O(\mathbf{r})$$

Object and probe updates from the minimization of the cost function[2]:

$$\varepsilon = \|\Psi - \Psi^0\|^2 = \sum_j \sum_r |\psi_j(\mathbf{r}) - P^0(\mathbf{r}-\mathbf{r}_j)O^0(\mathbf{r})|^2$$

$$\frac{\partial \varepsilon}{\partial O^0} = 0: \; O^0(\mathbf{r}) = \frac{\sum_j \psi_j(\mathbf{r})P^*(\mathbf{r}-\mathbf{r}_j)}{\sum_j |P(\mathbf{r}-\mathbf{r}_j)|^2} \qquad \frac{\partial \varepsilon}{\partial P^0} = 0: \; P^0(\mathbf{r}) = \frac{\sum_j \psi_j(\mathbf{r}+\mathbf{r}_j)O^*(\mathbf{r}+\mathbf{r}_j)}{\sum_j |O(\mathbf{r}+\mathbf{r}_j)|^2}$$

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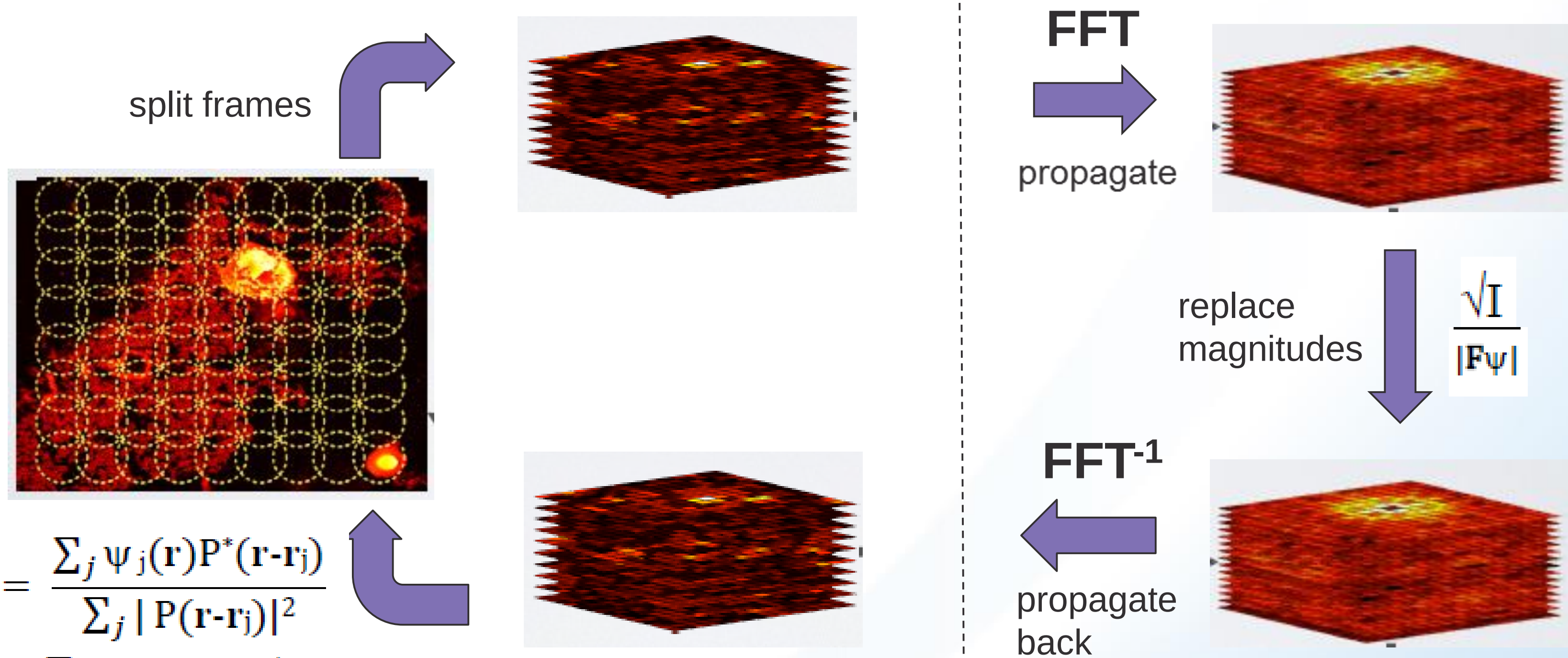
(1) V. Elser, Phase retrieval by iterated projections, J. Opt. Soc Am. A, 2003

(2) P. Thibault et al. Probe retrieval in ptychographic coherent diffractive imaging, Ultramicroscopy, 109, 2009

Ptychography Approach (in pictures*)

Sample space | *Detector space*

$$\pi_o(\psi): \psi \rightarrow P(\mathbf{r}\text{-}\mathbf{r}_j)O(\mathbf{r})$$



$$O^0(\mathbf{r}) = \frac{\sum_j \psi_j(\mathbf{r})P^*(\mathbf{r}\text{-}\mathbf{r}_j)}{\sum_j |P(\mathbf{r}\text{-}\mathbf{r}_j)|^2}$$

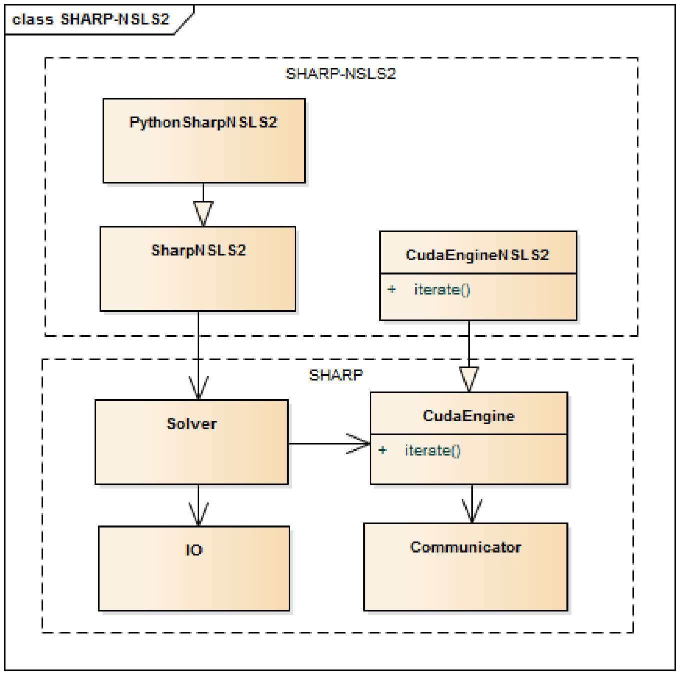
$$P^0(\mathbf{r}) = \frac{\sum_j \psi_j(\mathbf{r}+\mathbf{r}_j)O^*(\mathbf{r}+\mathbf{r}_j)}{\sum_j |O(\mathbf{r}+\mathbf{r}_j)|^2}$$

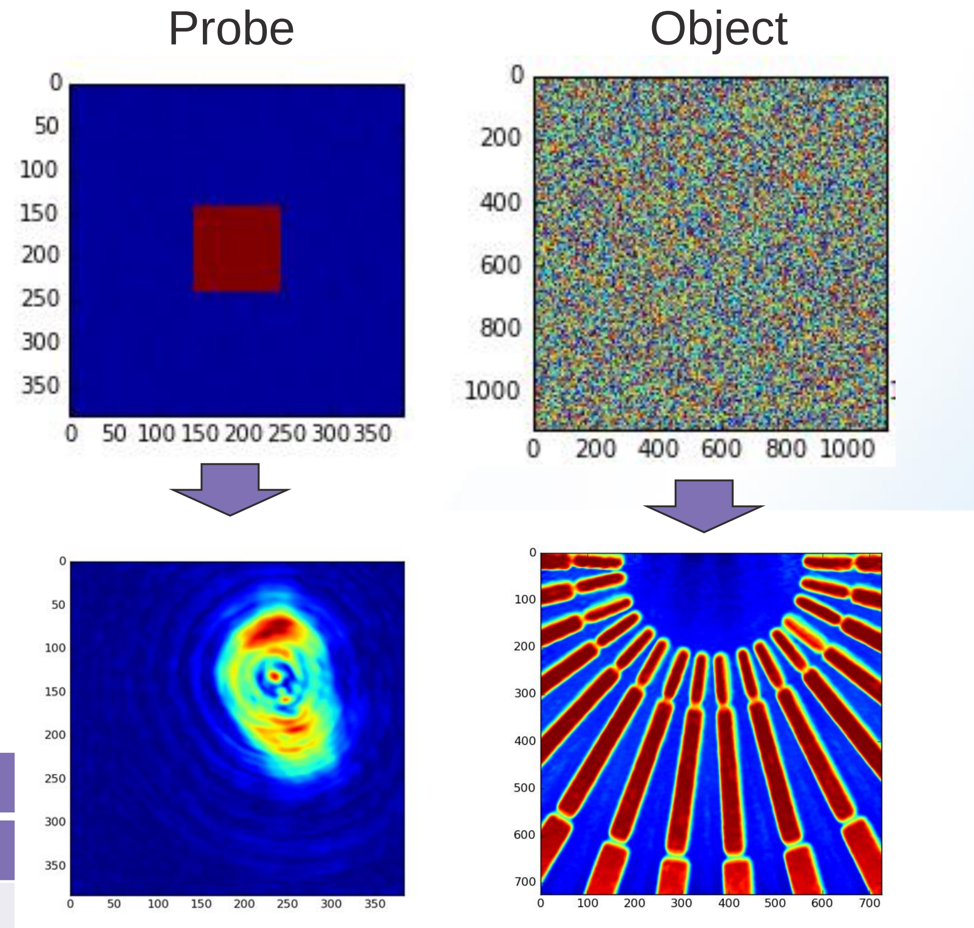
$$\pi_a(\psi): \psi \rightarrow \mathbf{F}^* \frac{F\psi}{|F\psi|}\sqrt{I}$$

S. Marchesini, Fast Scalabale methods for ptychographic imaging, SHARP workshop, LBNL, Oct 8, 2014

SHARP GPU-Based Solver and NSLS-II Application

SHARP-NSLS2

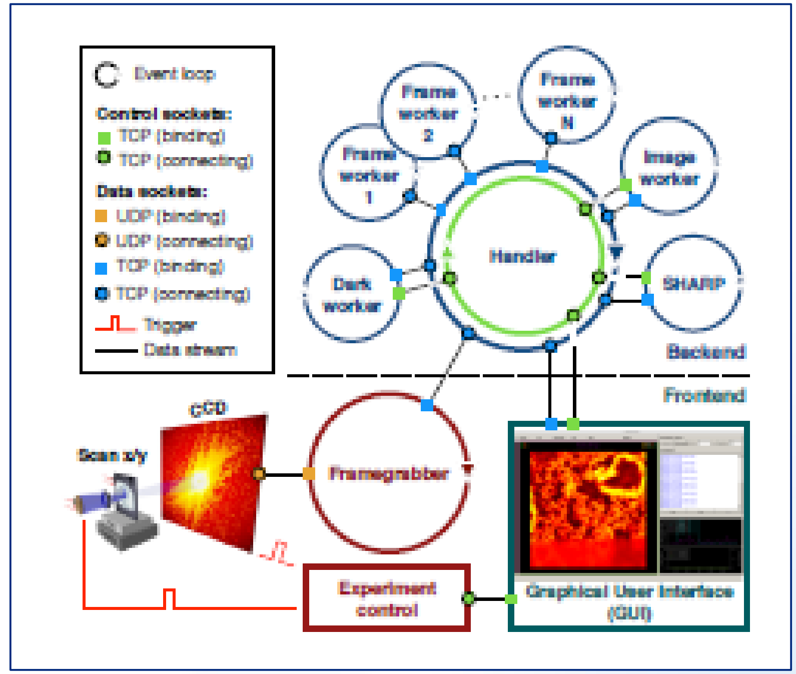


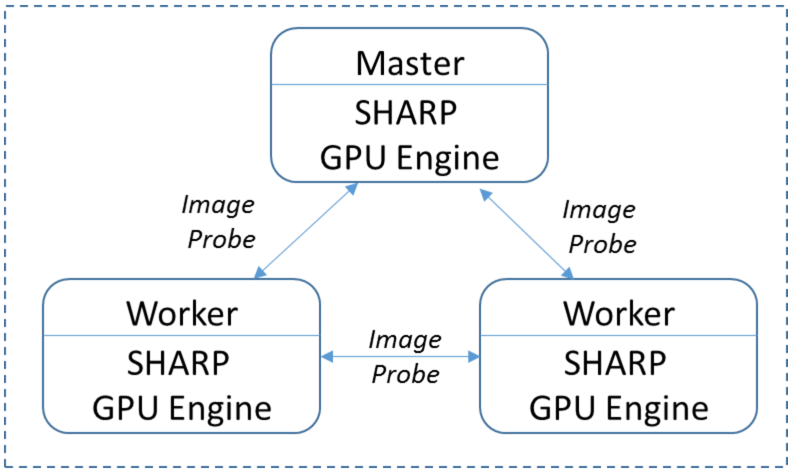


Functions	Time, s	
	256 frames	512 frames
Modulus & overlap projections	0.06	0.12
Probe update	0.025	0.05
Object update	0.03	0.06

Multi-GPU Approach

ALS Streaming Pipeline[1]





NSLS-II Spark-based SciDriver[2]

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(1) S. Marchesini et al. SHARP: a distributed, GPU-based ptychographic solver, LBNL-1003977, 2016

(2) N. Malitsky and N. D'Imperio, SciDriver: Driving Beamline Streams with HPC Applications, BNL LDRD Proposal, 2016

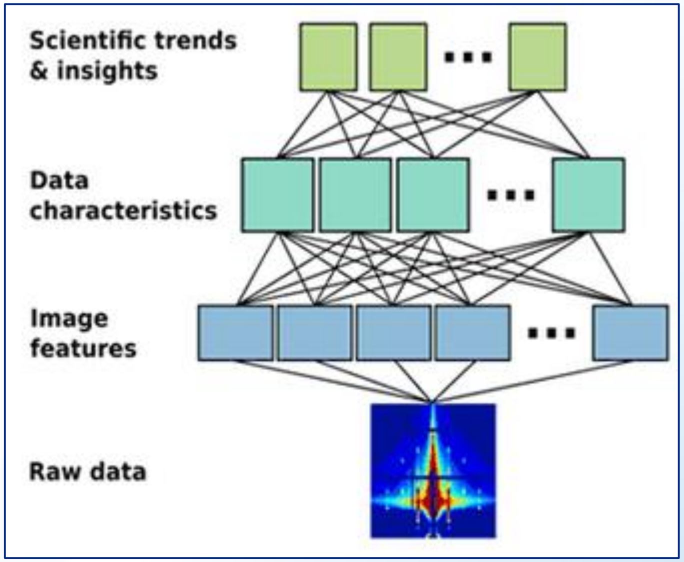
SPARK-BASED DISTRIBUTED DEEP LEARNING SOLVERS

Deep Learning Approach – 1 of 2

Deep learning is an active area of machine learning, achieving a state-of-the-art performance in multiple application domains, ranging from visual object recognition to reinforcement learning. The major category of methods is based on multi-layer (deep) architectures using the convolution neural network model.

A brief (and incomplete) history of the convolution neural network model:

- D. H. Hubel and T. N. Wiesel, “Receptive fields, binocular interactions, and functional architecture in the cat’s visual cortex, “Journal of Physiology, vol. 160, 1962
- K. Fukushima, “Neocognitron: A self-organizing neural network model for a mechanism of pattern recognition unaffected by shift in position, “ Biological Cybernetics, vol. 36, 1980
- Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner, “Gradient-based learning applied to document recognition, “Proc. of the IEEE, vol. 86, 1998



K. Yager (CFN) and D. Yu (CSI), Deep Learning for Analysis of Materials Science Data, BNL

Deep Learning Approach – 2 of 2

- **DistBelief, Google:**

J. Dean et al. Large Scale Distributed Deep Networks, NIPS 2012

- **Caffe, UC Berkeley :** http://caffe.berkeleyvision.org/

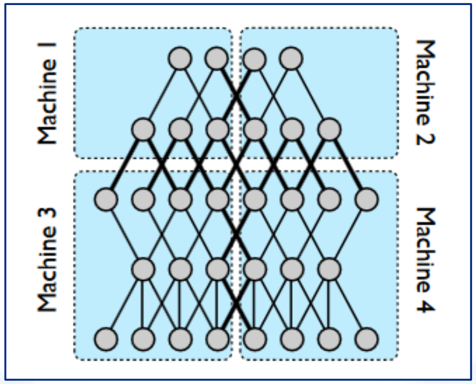
Y. Jia et al., Caffe: Convolution Architecture for Fast Feature Embedding, ACM International Conference on Multimedia, 2014

- **TensorFlow, Google:** https://www.tensorflow.org/

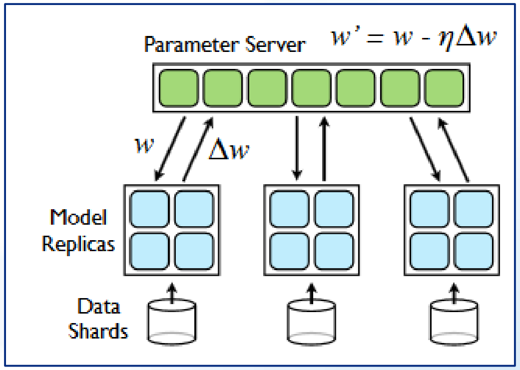
M. Abadi et al. TensorFlow: Large-Scale Machine Learning on Heterogeneous Distributed Systems, Preliminary White Paper, November 2015

Open source: Nov 2015, Distributed version: April 2016

Model Parallelism



Data Parallelism



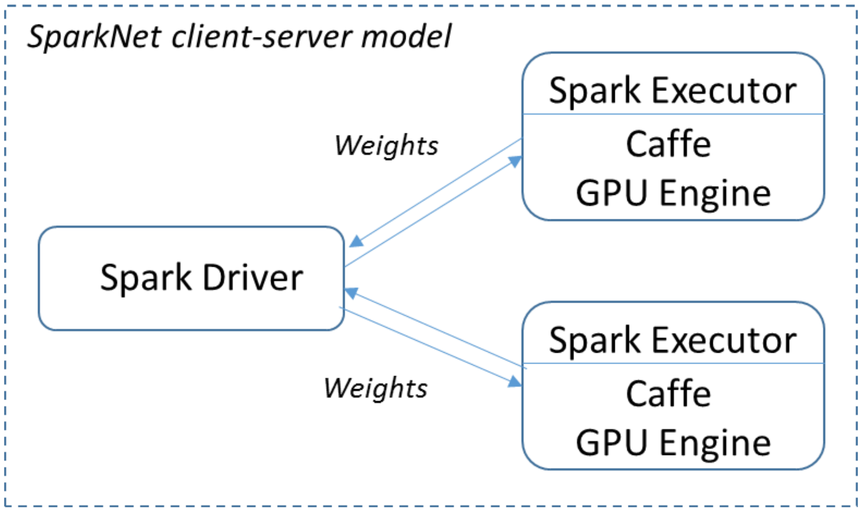
SparkNet*

Philipp Moritz, Robert Nishihara, Ion Stoica, and Michael Jordan. AMPLab, UC Berkeley

URL: https://github.com/amplab/SparkNet

API: Scala

Engine Wrapper: Scala/Java/C++



RDDs

```
var nets = trainData.foreachPartition( data => {
  var net = Net (…)
  net.setTrainingData(data)
  net })

var weights = initialWeights (…)

for ( i <- 1 to 1000){

   var broadcastWeights = broadcast(weights)

   nets.map(net => net.setWeights(broadcastWeights.value))

   weights = nets.map (net => {
         net.train (50)
         net.getWeights() }).mean()
}
```

from Driver to Workers

from Workers to Driver

Fragment of the Driver script*

P. Moritz, R. Nishihara, I. Stoica, and M. Jordan. SparkNet: Training Deep Networks in Spark, ICLR, 2016

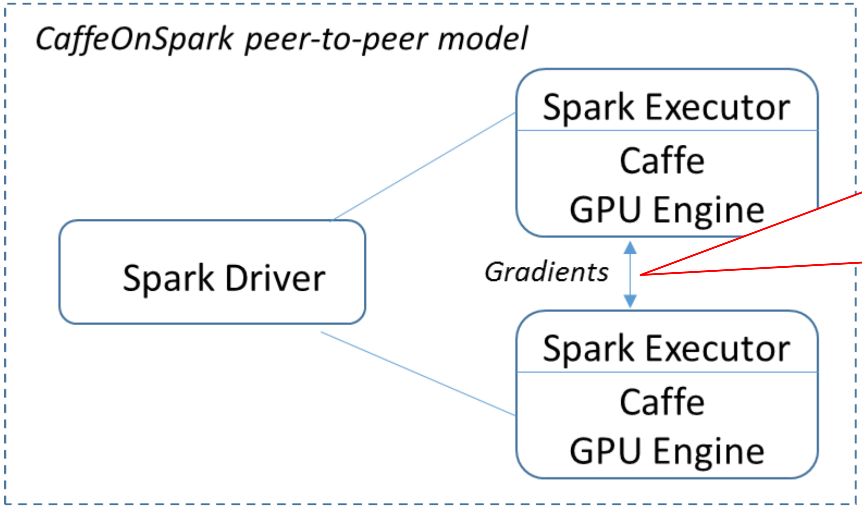
CaffeOnSpark*

Andy Feng, Jun Shi, and Mridul Jain. Yahoo Big ML Team

URL: https://github.com/yahoo/CaffeOnSpark

API: Python/Scala

Engine Wrapper: Scala/Java/C++



Inter-Worker Interface (C++):

- Ethernet/TCP
- InfiniBand/RDMA
- GPU or CPU

A. Feng, J. Shi, and Mridul Jain. CaffeOnSpark: Deep Learning on Spark Cluster, Spark Summit, June 2016

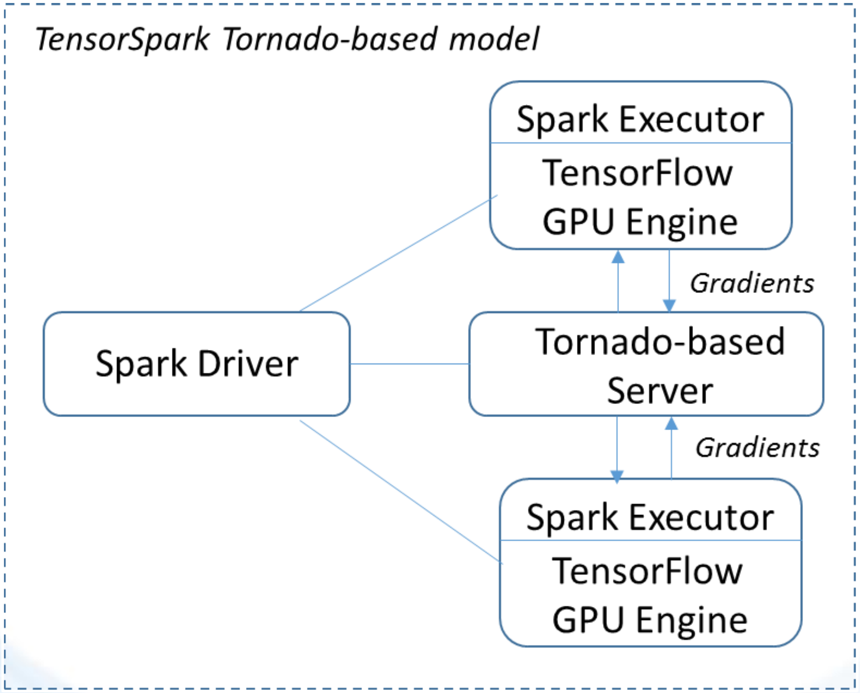
TensorSpark*

Christopher Nguyen, Chris Smith, Ushnish De, Vu Pham, and Nanda Kishore. Arimo

URL: https://github.com/adatao/tensorspark

API: Python

Engine Wrapper: Python/C++




```
# define a  worker function that calls the TensorFlow wrapper
def train_partition(partition):
      return TensorSparkWorker(…).train_partition(partition)

# access the Spark context
sc = pyspark.SparkContext(…)

# load data on distributed workers and cache them in memory
training_rdd = sc.textFile(…).cache()

# start the Tornado-based parameter server
param_server = ParameterServer(…)
param_server.start()

# start a training loop
for i in range(num_epochs):
      # run the train_partition function on distributed workers
      training_rdd.mapPartitions (train_partition).collect()
```

Fragment of the Driver script

C. Nguyen et al. Distributed TensorFlow on Spark: Scaling Google's Deep Learning Library, Spark Summit, February 2016

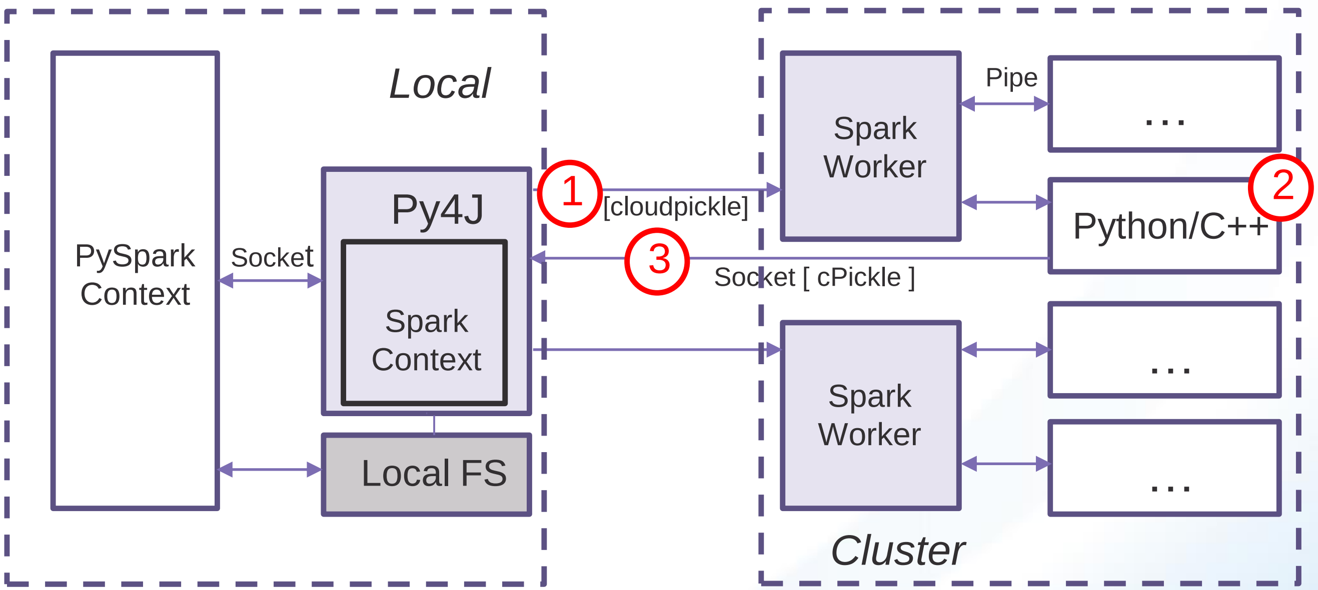
PySpark*

```
In [24]: def send_arrays(x):
             t1 = datetime.now();
             results = [];
             for i in range(0, 10) :
                 results.append(np.arange(1000000, dtype = np.float))
             t2 = datetime.now();
             print "create_arrays, length: ", len(results), " time: ", (t2 - t1)
             return results
```

create_arrays, length: 10 time: 0:00:00.038749

```
In [25]: t1 = datetime.now()
         send_arrays_rdd = sc.parallelize(xrange(1, partitions + 1), partitions).map(send_arrays);
         mfs = send_arrays_rdd.collect();
         t2 = datetime.now();
         print "collect, length: ", len(mfs[0]), "time: ", (t2 - t1);
```

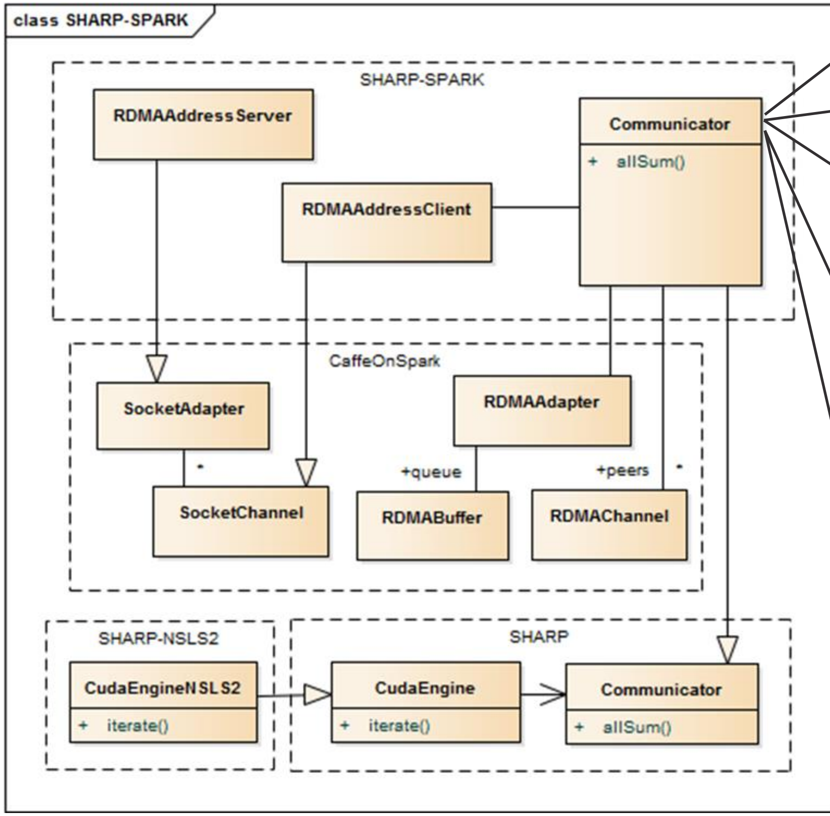
```
collect, length:  10 time:  0:00:01.126674
```



https://cwiki.apache.org/confluence/display/SPARK/PySpark+Internals

SHARP-SPARK

SHARP-SPARK



Benchmark results on 4 nodes

Approach	Time, s
MPI Allreduce based on MVAPICH2	0.013
SHARP-SPARK based on the CaffeOnSpark library	0.016

```
def wf(args):

    comm = Communicator.createCommunicator(args['rank'], args['size'])

    # 1. allocate buffers used in the peer-to-peer communication
    imageSize = 2*1000000
    comm.allocate(imageSize*4)

    # 2. connect to the address server and
    # exchange the RDMA addresses
    comm.connect(args['addr'])

    # define a local array (e.g. image)
    a = np.zeros(imageSize, dtype=np.float32)
    a[imageSize-1] = 1.0

    # 3. sum peers' arrays for several iterations
    t1 = datetime.now()

    for i in range(0, 10):
        comm.allSum(a)

    t2 = datetime.now()

    # prepare and return the benchmark results
    out = {
        'a' : a[imageSize-1],
        'time' : (t2-t1),
    }

    comm.release()

    return out
```

Worker's function of the benchmark application

Summary

- Outlined Spark as an integrated platform for the Big Data and Big Computing applications at experimental facilities

- Presented the SHARP-SPARK application highlighting the MPI-oriented development of the Spark computational model

Acknowledgement

SHARP Team, CAMERA, LBNL: H. Krishnan, S. Marchesini, T. Perciano, J. Sethian, D. Shapiro

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HXN Group, NSLS-II, BNL: X. Huang

Control Group, NSLS-II, BNL: M. Cowan, L. Flaks, A. Heroux, K. Lauer, R. Petkus

Computational Science Lab, CSI, BNL: N. D' Imperio, D. Zhihua

Information Technology Division, BNL: R. Perez