BigData Analytics with Spark and Hadoop at OSC

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What is BigData

Bigdata is an evolving term that describes any voluminous amount of structured and unstructured data that has the potential to be mined for information.

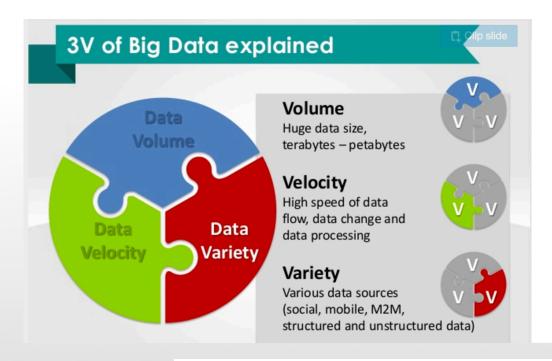
Bigdata generates value from the storage and processing of very large quantities of digital information that cannot be analyzed with traditional computing techniques

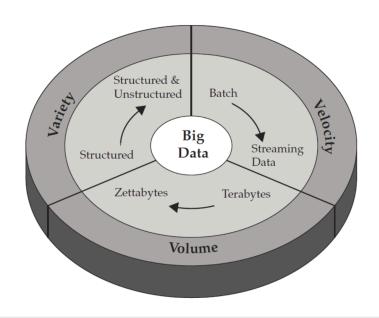
Helps to solve new problem or old problem in a better way





The 3V of Big Data





- ▶ Key enablers for the growth of "Big Data" are:
 - Increase of storage capacities
 - Increase of processing power
 - Availability of data



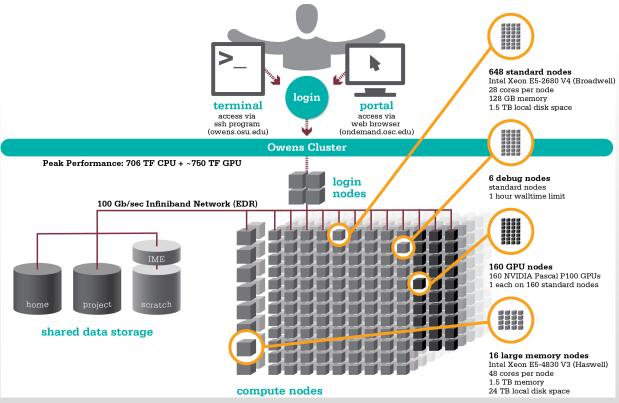
Data Analytical Tools

	Examples	Characteristics	Typical tools	Analytical methods
Small Data (megabytes)	Sales records, Customers database (small and medium companies)	Hundreds – thousands of records	Personal computer, Excel, R, other basic statistics software	Simple statistics
Large Data (gigabytes- terabytes)	Customer databases (big companies)	Millions of records, mostly structured data	Server workstation computer, Relational database systems, data warehouses	Advanced statistics, business intelligence, data mining,
Big Data (terabytes – petabytes)	Customer interactions (social media, mobile), multimedia (video, images, free text), location-based data, RFIM	Over millions of records, distributed, unstructured	Cloud, data centers, Distributed databases, NoSQL, Hadoop	MapReduce, Distributed File Systems



Data Analytical nodes@OSC

Owens' data analytics environment is comprised of 16 nodes, each with 48 CPU cores, 1.5TB of RAM and 24TB of local disk.



\$HOME:

500GB/per user 1.5TB or 24TB

Local disk:\$TMPDIR Backed up daily Not backed up Not backed up

/fs/scratch: 1200TB Permanent storage Temporary storage Temporary storage

/fs/project: Upon request 1-5TB Backed up daily 1-3 years



OSC OnDemand ondemand.osc.edu

- 1: User Interface
 - Web based
 - Usable from computers, tablets, smartphones
 - Zero installation
 - Single point of entry
 - User needs three things
 - ondemand.osc.edu
 - OSC Username
 - OSC Password
 - Connected to all resources at OSC

- 2: Interactive Services
 - File Access
 - Job Management
 - Visualization Apps
 - Desktop access
 - Single-click apps (Abaqus, Ansys, Comsol, Paraview)
 - Terminal Access

Tutorial available at osc.edu/ondemand

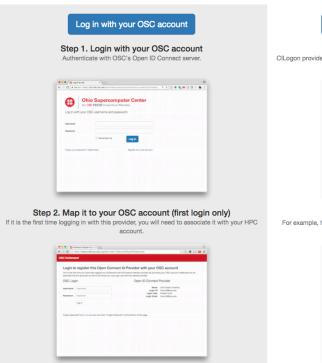


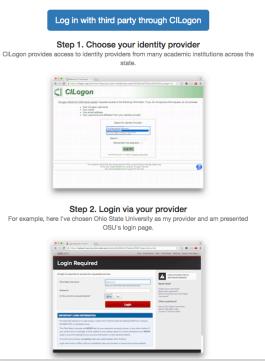
Go to https://ondemand.osc.edu/

OSC OnDemand

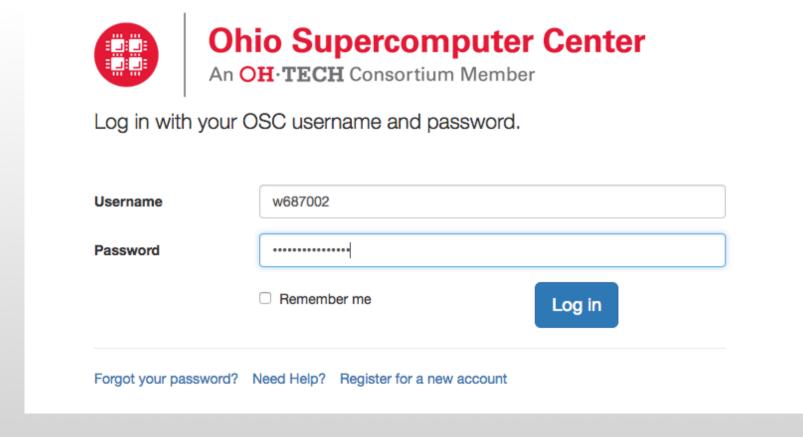
Login to OSC OnDemand

Log in with either your OSC Account or a third party account via ClLogon. If you don't have an OSC Account, register for one here.



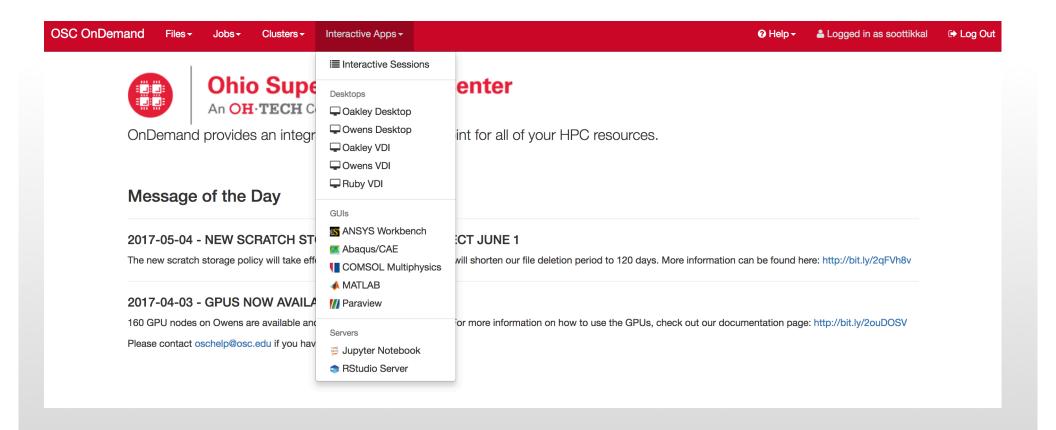
















Exercise-1

Login to OSC OnDemand



Data Analytics@OSC

Python: A popular general-purpose, high-level programming language with numerous mathematical and scientific packages available for data analytics.

R: A programming language for statistical and machine learning applications with very strong graphical capabilities.

MATLAB: A full featured data analysis toolkit with many advanced algorithms readily available.

Spark and Hadoop: Frameworks for running map reduce algorithms

Intel Compilers: Compilers for generating optimized code for Intel CPUs.

Intel MKL: The Math Kernel Library provides optimized subroutines for common computation tasks such as matrix-matrix calculations.

Statistical software: Octave, Stata, FFTW, ScaLAPACK, MINPACK, sprng2



R and Rstudio

R is a language and environment for statistical computing and graphics. R provides a wide variety of statistical and graphical techniques and is highly extensible.

Availability:

The following versions of R are available on OSC systems:

VERSION	OAKLEY	OWENS
3.0.1	X	
3.1.3	X	
3.2.0	X	
3.3.1	X*	X
3.3.2		X*
3.4.0		X
3.4.2		X
3.5.0		X

Running R interactively

Set-up

In order to configure your environment for the usage of R, run the following command:

module load R

Using R

Once your environment is configured, R can be started simply by entering the following command:

R

For a listing of command line options, run:

R --help

Batch Usage

```
#PBS -N R_ExampleJob
#PBS -l nodes=1:ppn=12
```

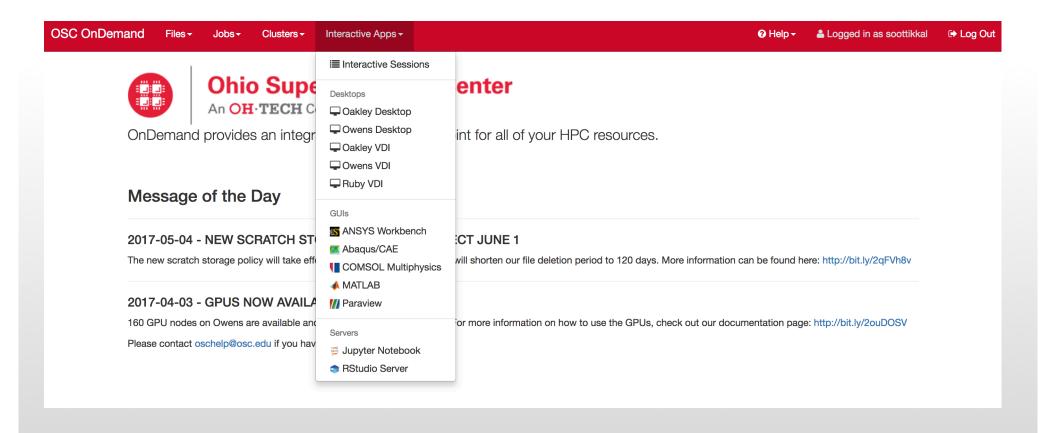
module load R
cd \$PBS_O_WORKDIR
cp in.dat test.R \$TMPDIR
cd \$TMPDIR

R CMD BATCH test.R test.Rout

cp test.Rout \$PBS_O_WORKDIR

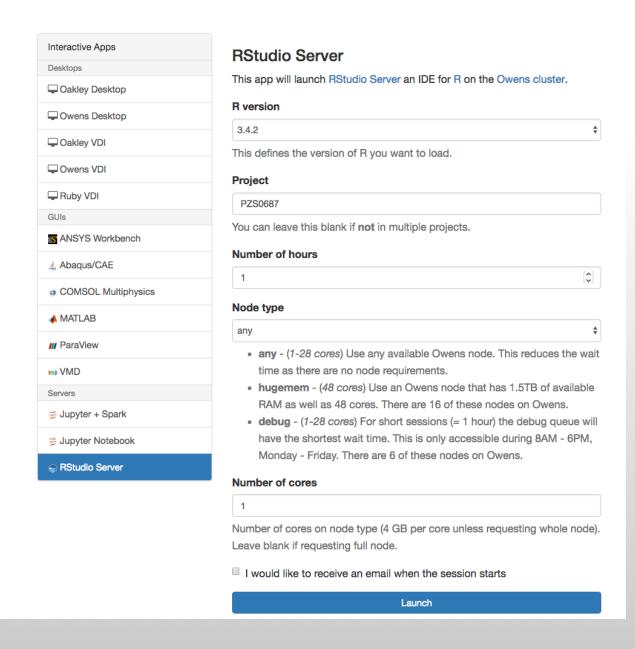


Rstudio on Ondemand



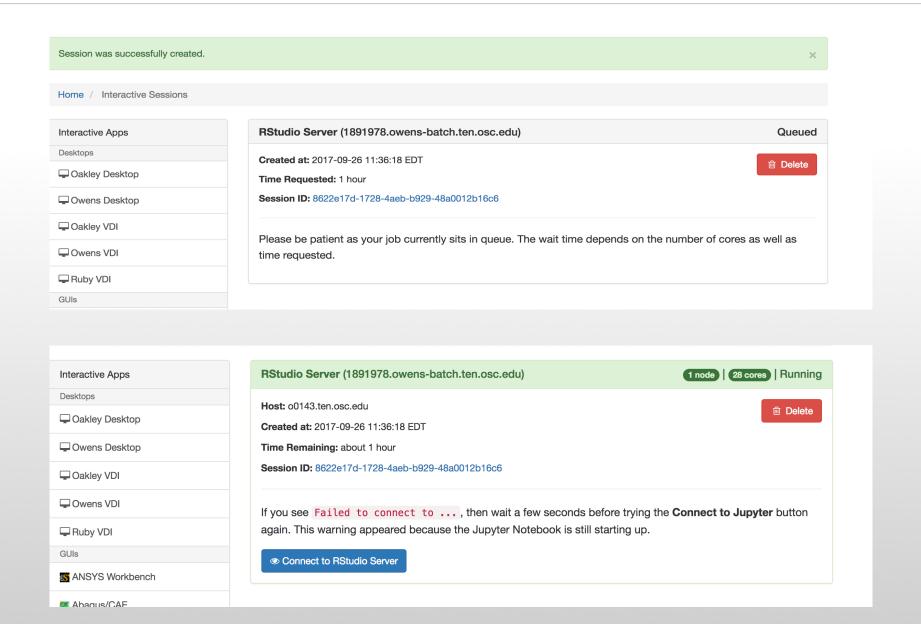






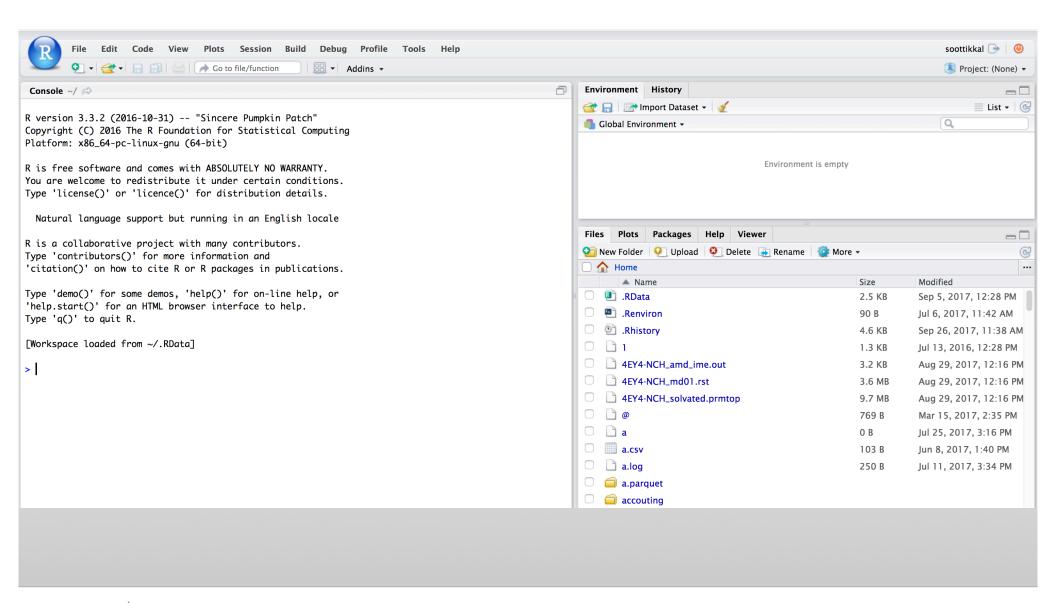




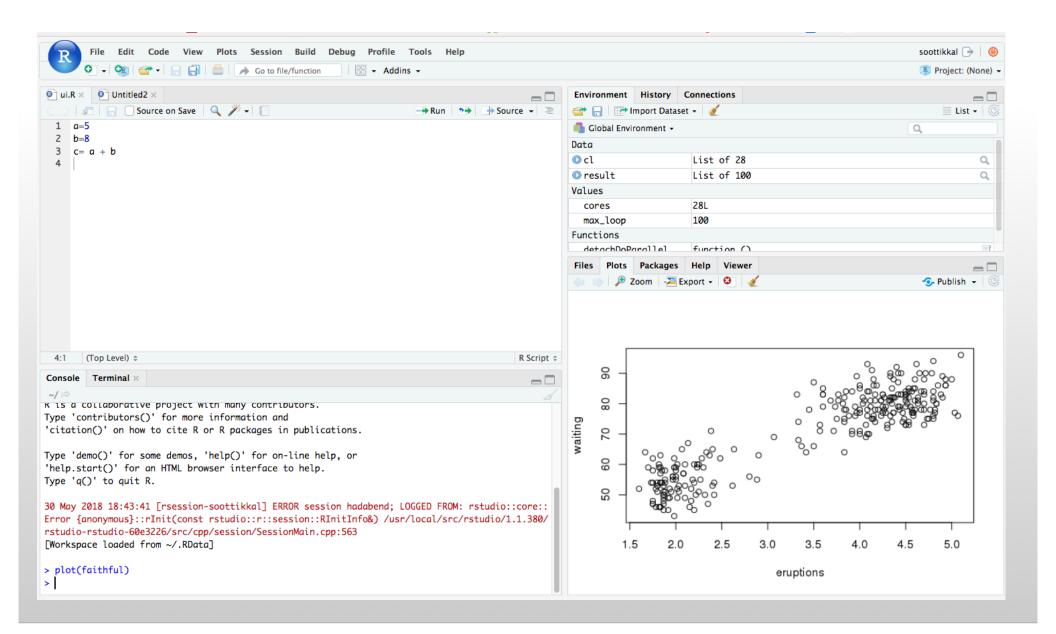














Exercise-2

Launching Rstudio App





Apache Spark

Apache Spark is an open source cluster computing framework originally developed in the AMPLab at University of California, Berkeley but was later donated to the Apache Software Foundation where it remains today. In contrast to Hadoop's disk-based analytics paradigm, Spark has multi-stage in-memory analytics.

Speed

Run programs up to 100x faster than Hadoop MapReduce in memory, or 10x faster on disk.

Spark has an advanced DAG execution engine that supports cyclic data flow and in-memory computing.

120 110 Hadoop Spark

Logistic regression in Hadoop and Spark

Ease of Use

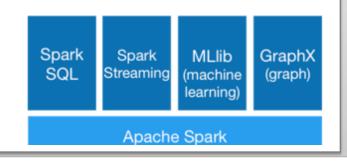
Write applications quickly in Java, Scala, Python, R.

Spark offers over 80 high-level operators that make it easy to build parallel apps. And you can use it *interactively* from the Scala, Python and R shells.

Generality

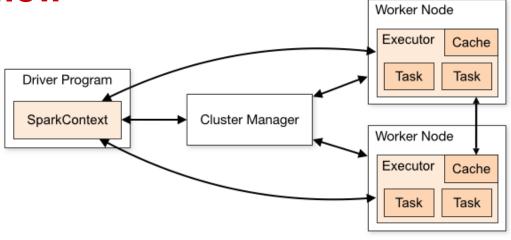
Combine SQL, streaming, and complex analytics.

Spark powers a stack of libraries including SQL and DataFrames, MLlib for machine learning, GraphX, and Spark Streaming. You can combine these libraries seamlessly in the same application.





Spark workflow



Spark applications run as independent sets of processes on a cluster, coordinated by the SparkContext object in your main program (called the driver program).

Requires cluster managers which allocate resources across applications.

Once connected, Spark acquires executors on nodes in the cluster, which are processes that run computations and store data for your application.

Next, it sends your application code (defined by JAR or Python files passed to SparkContext) to the executors. Finally, SparkContext sends tasks to the executors to run.



RDD- Resilient Distributed Datasets

RDD (Resilient Distributed Dataset) is the main logical data unit in Spark. They are

- Distributed and partitioned
- ◆ Stored in memory
- ◆ Immutable
- Partitions recomputed on failure

RDD- Transformations and Actions

Transformations are executed on demand. That means they are computed lazily. Eg: filter, join, sort

Actions return final results of RDD computations. Actions triggers execution using lineage graph to load the data into original RDD, carry out all intermediate transformations and return final results to Driver program or write it out to file system. Eg: collect(), count(), take()

RDD Operations

Transformations

```
map(func)
flatMap(func)
filter(func)
groupByKey()
reduceByKey(func)
mapValues(func)
```

Actions

```
take(N)
count()
collect()
reduce(func)
takeOrdered(N)
top(N)
```

Interactive Analysis with the Spark Shell

\$SPARK_HOME/bin/pyspark # Opens SparkContext

1. Create a RDD

>>> data = sc.textFile("README.md")

2. Transformation of RDD

>>>linesWithSpark = data.filter(lambda line: "Spark" in line)

3. Action on RDD

>>> linesWithSpark.count() # Number of items in this RDD 12

4. Combining Transformation and Actions

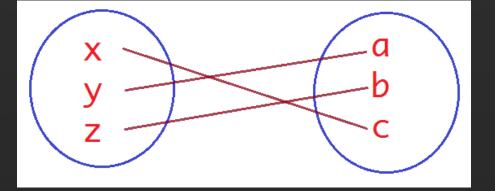
>>> data.filter(lambda line: "Spark" in line).count() # How many lines contain "Spark"?



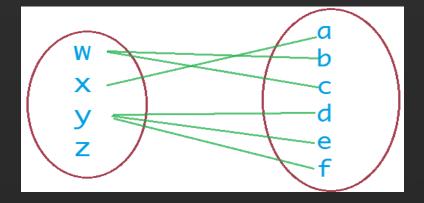
Word count Example

Map: One element in input gets mapped to only one element in output. Flatmap: One element in input maps to zero or more elements in the output.

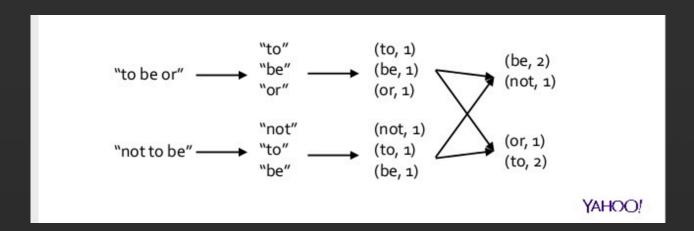
Мар



Flatmap



Word count Example



>>>wordCounts = data.flatMap(lambda line: line.split()).map(lambda word: (word,1)).reduceByKey(lambda a, b: a+b)

>>> wordCounts.collect()



Spark documentation at OSC

https://www.osc.edu/resources/available_software/software_list/spark

versions

The following versions of Spark are available on OSC systems:

VERSION	OAKLEY	OWENS
1.5.2	X	
1.6.1	x	
2.0.0	X*	X*
2.1.0		X

Set-up

In order to configure your environment for the usage of Spark, run the following command:

module load spark

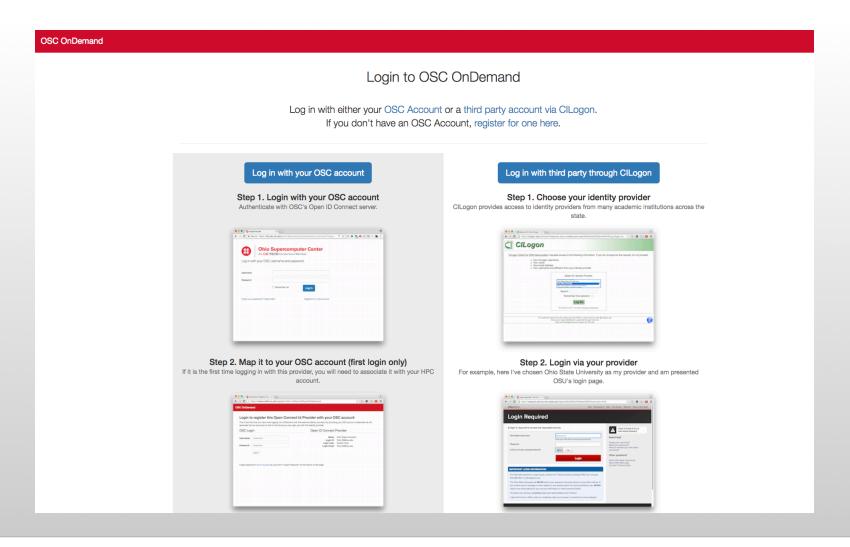
In order to access a particular version of Spark, run the following command

module load spark/2.0.0



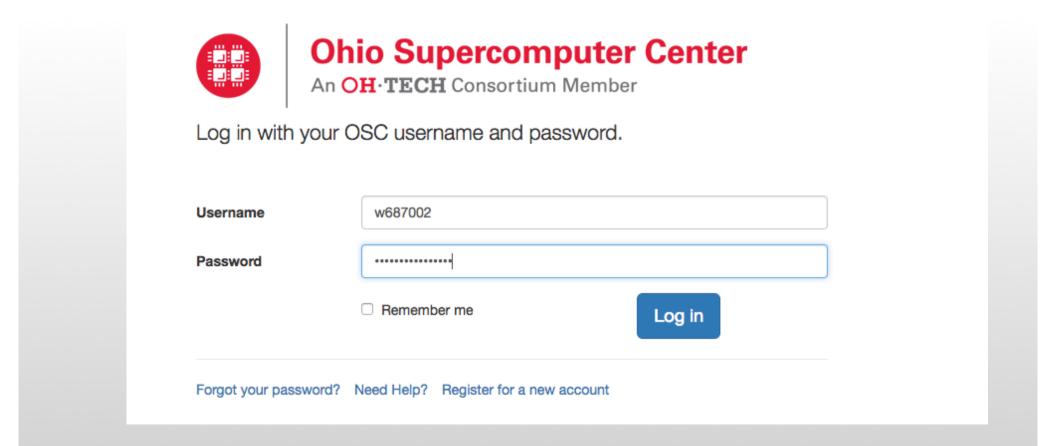
Running Spark interactively: Jupyter+Spark App

Go to https://ondemand.osc.edu/

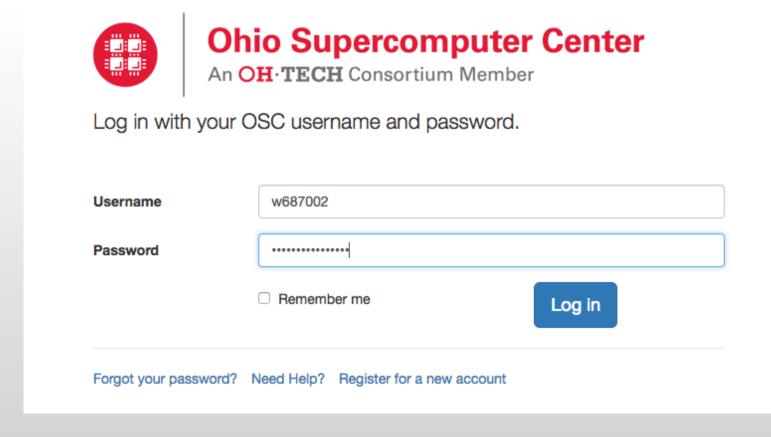




Log on with your OSC credentials.



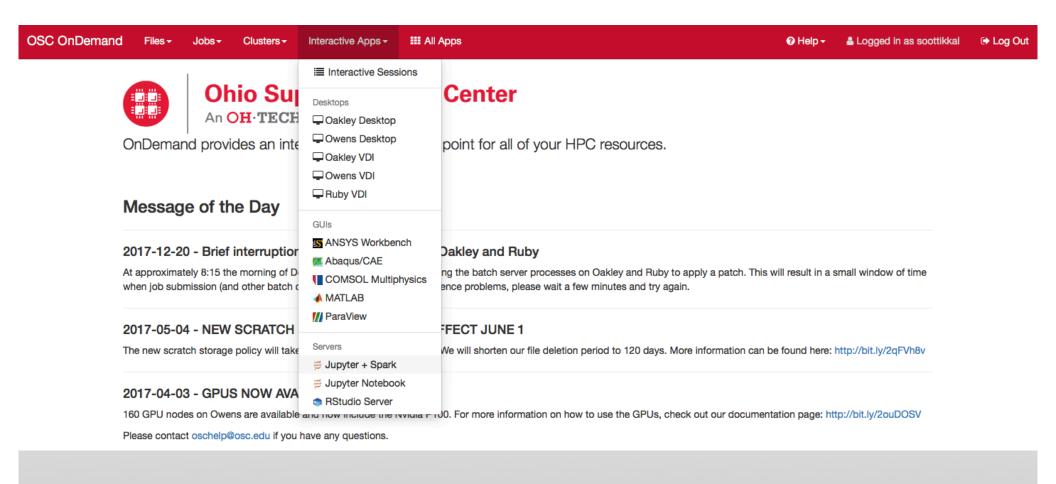








Choose Jupyter+Spark app from the Interactive Apps option.







Home / My Interactive Sessions / Jupyter + Spark

Interactive Apps →

Interactive Apps
Desktops
☐ Oakley Desktop
☐ Owens Desktop
☐ Oakley VDI
☐ Owens VDI
Ruby VDI
GUIs
S ANSYS Workbench
Abaqus/CAE
COMSOL Multiphysics
♠ MATLAB
ParaView
Servers
Jupyter + Spark
≅ Jupyter Notebook
RStudio Server

Jupyter + Spark

This app will launch a Jupyter Notebook server using Python as well as an Apache Spark cluster on the Owens cluster.

Project

PZS0687

You can leave this blank if not in multiple projects.

Number of hours

5

Number of nodes

2

Node type

any

- any (28 cores) Use any available Owens node. This reduces the wait time as there are no node requirements.
- hugemem (48 cores) Use an Owens node that has 1.5TB of available RAM as well as 48 cores. There are 16 of these nodes on Owens.

Number of workers per node

1

This describes how the cores and memory are divvied up on the node (useful to reduce memory allocated for each worker). Should be a multiple of the number of cores on the node you chose above. Do NOT exceed the number of cores on the node.

Only launch the driver on the master node.

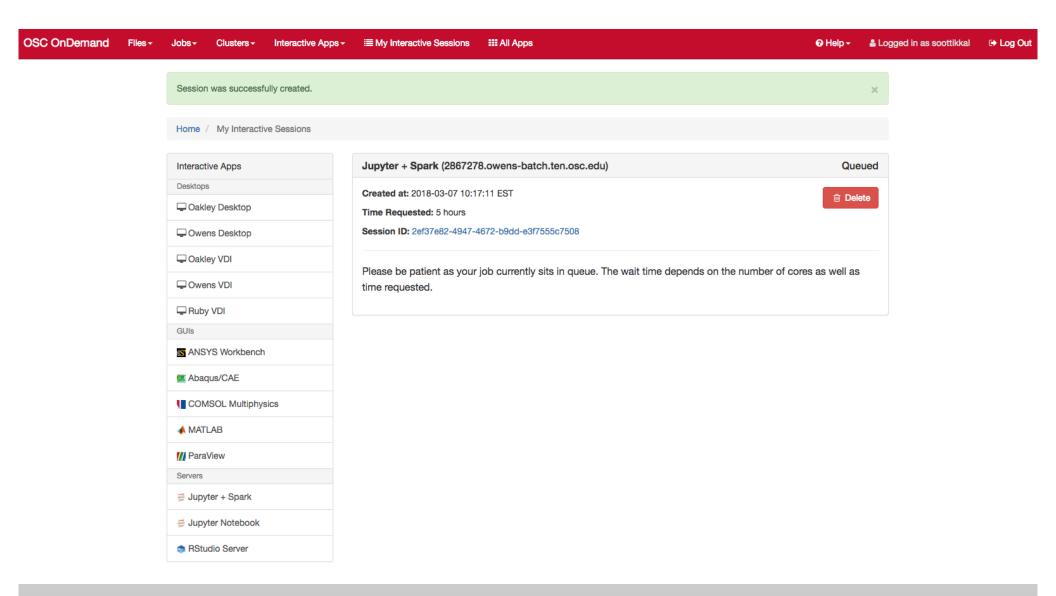
This is typically used for .collect and .take operations that require a large amount of memory allocated (> 2GB) for the driver process.

Include access to OSC tutorial/workshop notebooks.

☐ I would like to receive an email when the session starts

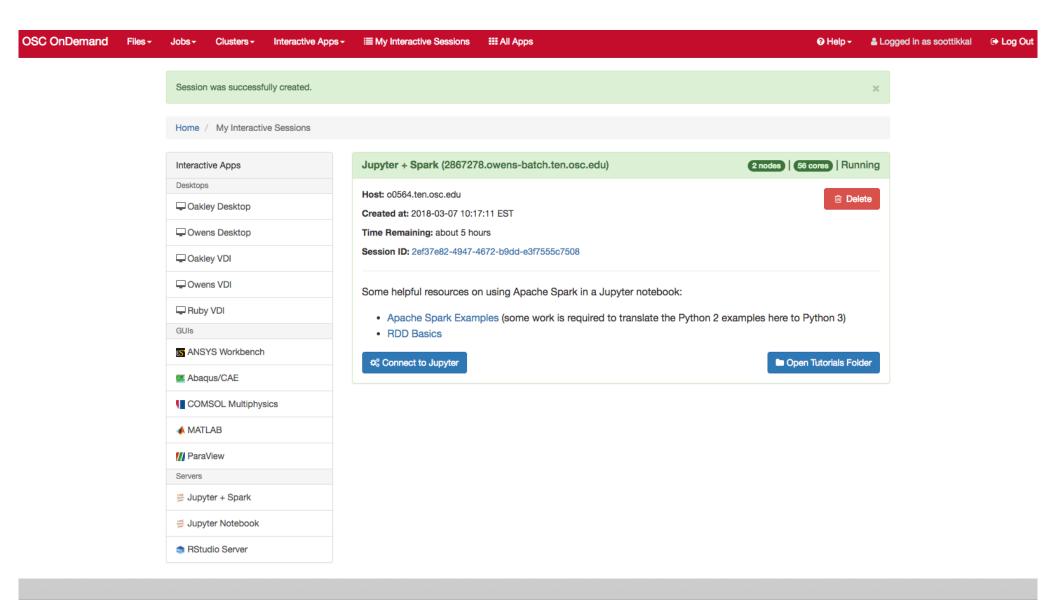
Launch

^{*} All Jupyter + Spark session data is generated and stored under the user's home directory in the corresponding data root directory.













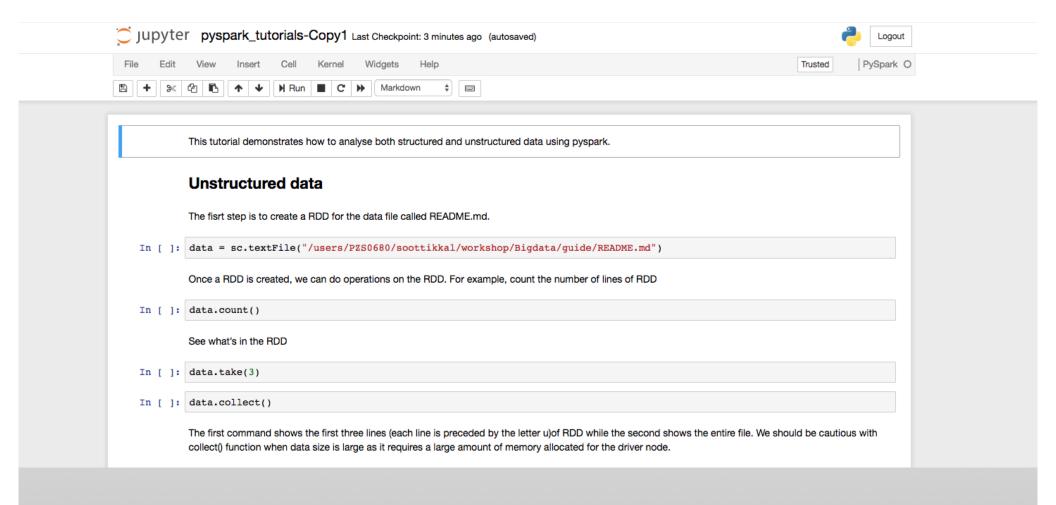
You will see a file called pyspark_tutorials.ipynb. Please check on the file and click on duplicate to make a copy of the file.



You will see a new file pyspark_tutorials-Copy1.ipynb is created. Double-click on the pyspark_tutorials-Copy1.ipynb file will launch Jupyter interface for Spark to proceed with the tutorials.











Exercise-3 Launching Jupyter + Spark App

https://www.osc.edu/content/la unching_jupyter_spark_app



Spark RDD

In this example, we are couting how many times each word appears in a file called README.md. The first step is to create a RDD from the data file called README.md. We will do some simple operations like count, take, collect on the RDD. Then we will use transformations like filter, flatmap and map to get the wordcount.

```
In [ ]: data = sc.textFile("/users/PZS0645/support/workshop/Bigdata/README.md")
```

Once a RDD is created, we can do operations on the RDD. For example, count the number of lines of RDD

```
In [ ]: data.count()
In [ ]: #See what's in the RDD
data.take(3)
In [ ]: data.collect()
```

The first command shows the first three lines (each line is preceded by the letter u)of RDD while the second shows the entire file. We should be cautious with collect() function when data size is large as it requires a large amount of memory allocated for the driver node to collect entire data

```
In [ ]: #Check the data type
type(data)
```

Next we'll do a simple transformation: filter all the lines with "Spark" in them and count such lines.

```
In [ ]: linesWithSpark = data.filter(lambda line: "Spark" in line)
In [ ]: linesWithSpark.count()
```



Spark DataFrame

Making a Simple DataFrame from a Tuple List.

```
In [34]: # Make a tuple list
         a_list = [('a', 1), ('b', 2), ('c', 3)]
In [35]: # Create a Spark DataFrame, without supplying a schema value
         df from list no schema = \
         sqlContext.createDataFrame(a list)
In [36]: # Print the DF object
         print (df_from_list_no_schema)
         DataFrame[_1: string, _2: bigint]
In [37]: # Print a collected list of Row objects
         print (df_from_list_no_schema.collect())
         [Row(_1='a', _2=1), Row(_1='b', _2=2), Row(_1='c', _2=3)]
In [38]: # Show the DataFrame
         df_from_list_no_schema.show()
```



Spark SQL

Inorder to run SparkSQL querries, we have to register the dataframe as table.

```
In [ ]: data.registerTempTable("interactions")

Now we can querry on the table called interactions based on conditions. For example, select tcp network interactions with more than 1 second duration and no transfer from destination

In [ ]: tcp = sqlContext.sql(" SELECT duration, dst_bytes FROM interactions WHERE protocal_type ='tcp' AND duration>1000 AND ds-
In [ ]: tcp.show(5)
```

Spark Mllib

- 1. Logistic regression: to predict a binary response
- 2. Kmeans clustering: to clusters the data points into a predefined number of clusters

Exercise-4

Spark Interactive Analytics





Running Spark interactively in batch

To run Spark interactively, but in batch on Owens please run the following command,

```
qsub -I -l nodes=4:ppn=28 -l walltime=01:00:00
```

When your interactive shell is ready, please launch spark cluster using the pbs-spark-submit script

```
pbs-spark-submit
```

You can then launch the interface for pyspark as follows,

```
pyspark --master spark://nodename.ten.osc.edu:7070
```

```
Python 2.7.5 (default, Oct 11 2015, 17:47:16)
[GCC 4.8.3 20140911 (Red Hat 4.8.3-9)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
Using Spark's default log4j profile: org/apache/spark/log4j-defaults.properties
Setting default log level to "WARN".
To adjust logging level use sc.setLogLevel(newLevel).
17/02/23 10:16:30 WARN NativeCodeLoader: Unable to load native-hadoop library for your platform... using builtin-java classes where applicable Welcome to
```

Using Python version 2.7.5 (default, Oct 11 2015 17:47:16) SparkSession available as 'spark'. >>> ■



Running Spark non-interactively

Using Spark

In order to run Spark in batch, reference the example batch script below. This script requests 6 node on the Oakley cluster for 1 hour of walltime. The script will submit the pyspark script called test.py using pbs-spark-submit command into the PBS queue.

```
#PBS -N Spark-example
#PBS -l nodes=6:ppn=12
#PBS -1 walltime=01:00:00
module load spark
cd $PBS_O_WORKDIR
cp test.py $TMPDIR
cd $TMPDIR
pbs-spark-submit test.py > test.log
cp * $PBS_O_WORKDIR
```



Running Spark using PBS script

1. Create an App in python: stati.py

```
from pyspark import SparkContext
import urllib
f = urllib.urlretrieve ("http://kdd.ics.uci.edu/databases/kddcup99/kddcup.data.gz","kddcup.data.gz")
data file = "./kddcup.data.gz"
sc = SparkContext(appName="Stati")
raw data = sc.textFile(data file)
import numpy as np
def parse interaction(line):
    line split = line.split(",")
    symbolic indexes = [1,2,3,41]
    clean line split=[item for i, item in enumerate(line split) if i not in symbolic indexes]
    return np.array([float(x) for x in clean line split])
vector data=raw data.map(parse interaction)
from pyspark.mllib.stat import Statistics
from math import sgrt
summary = Statistics.colStats(vector data)
print ("Duration Statistics:")
print (" Mean %f" % (round(summary.mean()[0],3)))
print ("St. deviation : %f"%(round(sqrt(summary.variance()[0]),3)))
print (" Max value: %f"%(round(summary.max()[0],3)))
print (" Min value: %f"%(round(summary.min()[0],3)))
```



2. Create a PBS script: stati.pbs

```
#PBS -N spark-statistics
#PBS -l nodes=18:ppn=28
#PBS -l walltime=00:10:00
module load spark/2.0.0
cp stati.py $TMPDIR
cd $TMPDIR
pbs-spark-submit stati.py > stati.log
cp * $PBS_0_WORKDIR
```

3. Run Spark job

qsub stati.pbs

4. Output: stati.log

```
sync from spark://n0381.ten.osc.edu:7077
starting org.apache.spark.deploy.master.Master, logging to
/nfs/15/soottikkal/spark/kdd/spark-soottikkal-org.apache.spark.deploy.master.Master-1-
n0381.ten.osc.edu.out
failed to launch org.apache.spark.deploy.master.Master:
full log in /nfs/15/soottikkal/spark/kdd/spark-soottikkal-
org.apache.spark.deploy.master.Master-1-n0381.ten.osc.edu.out

Duration Statistics:
Mean 48.342000
St. deviation : 723.330000
Max value: 58329.000000
Min value: 0.000000
Total value count: 4898431.000000
Number of non-zero values: 118939.000000

SPARK MASTER=spark://n0381.ten.osc.edu:7077
```



Exercise-5 Spark non-interactive jobs

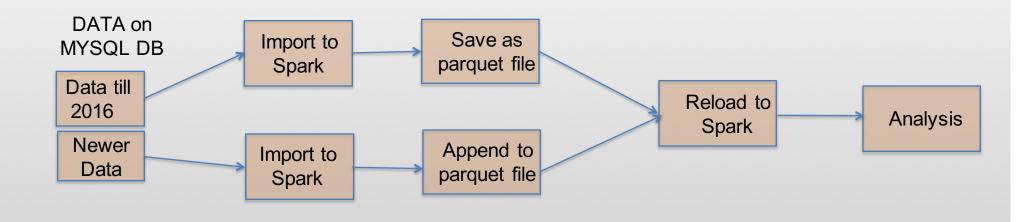
https://www.osc.edu/content/submitting_non_interactive_jobs

CASE STUDY

Data mining of historical jobs records of OSC's clusters

Aim: To understand client utilizations of OSC recourses.

Data: Historical records of every Job that ran on any OSC clusters that includes information's such as number of nodes, software, CPU time and timestamp.



Pyspark code for data analysis

#importing data

df=sqlContext.read.parquet("/fs/scratch/pbsacct/Jobs.parquet")
df.show(5)

+					+	+-	+
jobid	username	system	nproc	submit_date	end_date	jobname s	w_app queue
†							+
13780.owens-batch	3	owens	280	2016-09-28	2016-10-08	MMPCDH24EC1-3-2eq	namd parallel
13786.owens-batch	4	owens	96	2016-09-28	2016-10-05	FR181-011DS	foam parallel
13798.owens-batch	30	owens	252	2016-09-28	2016-10-03	TSRD-5-3-012DS	foam parallel
13800.owens-batch	30	owens	252	2016-09-28	2016-10-02	TSRD-5-3-013MSE	foam parallel
13804.owens-batch	30	owens	252	2016-09-28	2016-10-02	TSRD-5-3-014MSE	foam parallel
+							+

#Which types of queue is mostly used

df.select("jobid","queue").groupBy("queue").count().show()

#Which software is used most?

df.select("jobid","sw_app").groupBy

("sw_app").count().sort(col("count").desc()) .show()

#who uses gaussian software most?

df.registerTempTable("Jobs")

sqlContext.sql(" SELECT username FROM

Jobs WHERE sw_app='gaussian' ").show()

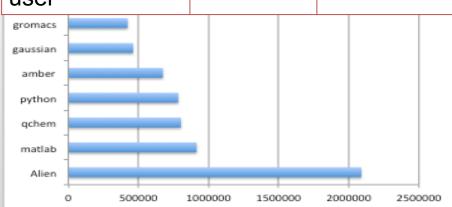
4.		
ļ	queue	count
+	debug serial montecarlo parallel hugemem largeparallel longserial dedicated	288174 12 41214 102 60 66
+		+

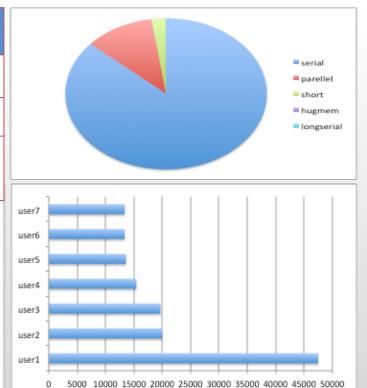
sw_app count
condor 40199 fastsimcoal 39535 null 36914 amber 35304 real_exe 31076 molcas 23695 vasp 18164 gadget 13880 bam 13189
hpl 9820



Results

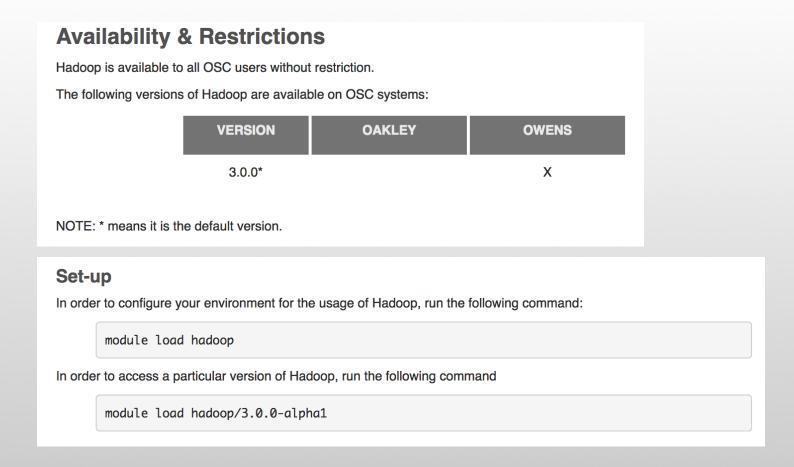
Statistics	MYSQL	SPARK
Job vs CPU	1 hour	5 sec
CPU vs Account	1.25 hour	5 sec
Walltime vs user	1.40 hour	5 sec





Running Hadoop at OSC

A Hadoop cluster can be launched within the HPC environment, but managed by the PBS job scheduler using Myhadoop framework developed by San Diego Supercomputer Center. (Please see http://www.sdsc.edu/~allans/MyHadoop.pdf)





Using Hadoop: Sample PBS Script

```
#PBS -N hadoop-example
#PBS -l nodes=6:ppn=12
#PBS -1 walltime=01:00:00
setenv WORK $PBS_O_WORKDIR
module load hadoop/3.0.0-alpha1
module load myhadoop/v0.40
setenv HADOOP_CONF_DIR $TMPDIR/mycluster-conf-$PBS_JOBID
cd $TMPDIR
myhadoop-configure.sh -c $HADOOP_CONF_DIR -s $TMPDIR
$HADOOP_HOME/sbin/start-dfs.sh
hadoop dfsadmin -report
hadoop dfs -mkdir data
hadoop dfs -put $HADOOP_HOME/README.txt data/
hadoop dfs -ls data
hadoop jar $HADOOP_HOME/share/hadoop/mapreduce/hadoop-mapreduce-examples-3.0.0-alpha1.jar
wordcount data/README.txt wordcount-out
hadoop dfs -ls wordcount-out
hadoop dfs -copyToLocal -f wordcount-out $WORK
$HADOOP_HOME/sbin/stop-dfs.sh
myhadoop-cleanup.sh
```





Using Hadoop: Sample PBS Script

```
#PBS -N hadoop-example
#PBS -l nodes=6:ppn=12
#PBS -1 walltime=01:00:00
setenv WORK $PBS_O_WORKDIR
module load hadoop/3.0.0-alpha1
module load myhadoop/v0.40
setenv HADOOP_CONF_DIR $TMPDIR/mycluster-conf-$PBS_JOBID
cd $TMPDIR
myhadoop-configure.sh -c $HADOOP_CONF_DIR -s $TMPDIR
$HADOOP_HOME/sbin/start-dfs.sh
hadoop dfsadmin -report
hadoop dfs -mkdir data
hadoop dfs -put $HADOOP_HOME/README.txt data/
hadoop dfs -ls data
hadoop jar $HADOOP_HOME/share/hadoop/mapreduce/hadoop-mapreduce-examples-3.0.0-alpha1.jar
wordcount data/README.txt wordcount-out
hadoop dfs -ls wordcount-out
hadoop dfs -copyToLocal -f wordcount-out $WORK
$HADOOP_HOME/sbin/stop-dfs.sh
myhadoop-cleanup.sh
```



Exercise-6 Hadoop jobs

https://www.osc.edu/content/submit ting_non_interactive_jobs





References

1. Spark Programming Guide

https://spark.apache.org/docs/2.0.0/programming-guide.html
-Programming with Scala, Java and Python

2. Data Exploration with Spark

http://www.cs.berkeley.edu/~rxin/ampcamp-ecnu/data-exploration-using-spark.html

3. Hadoop

http://hadoop.apache.org/

4. OSC Documentation

https://www.osc.edu/documentation/software_list/spark_documentation https://www.osc.edu/resources/available_software/software_list/hadoop



Thank you!

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