BigData Analytics with Spark and Hadoop at OSC

06/06/2018 OSC workshop Shameema Oottikkal Data Application Engineer Ohio Supercomputer Center email:soottikkal@osc.edu

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.

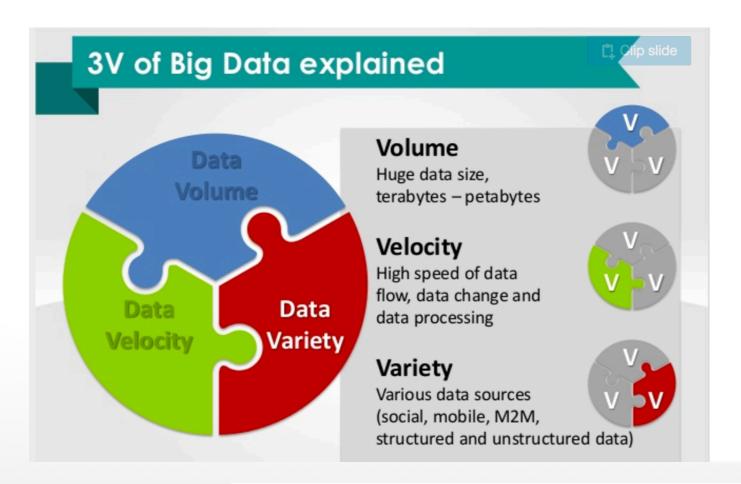
Bigdata generates value from the storage and processing of very large quantities of digital information that cannot be analyzed with traditional computing techniques

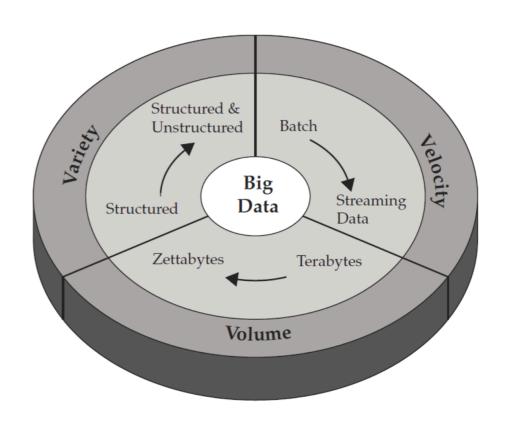
Helps to solve new problem or old problem in a better way





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

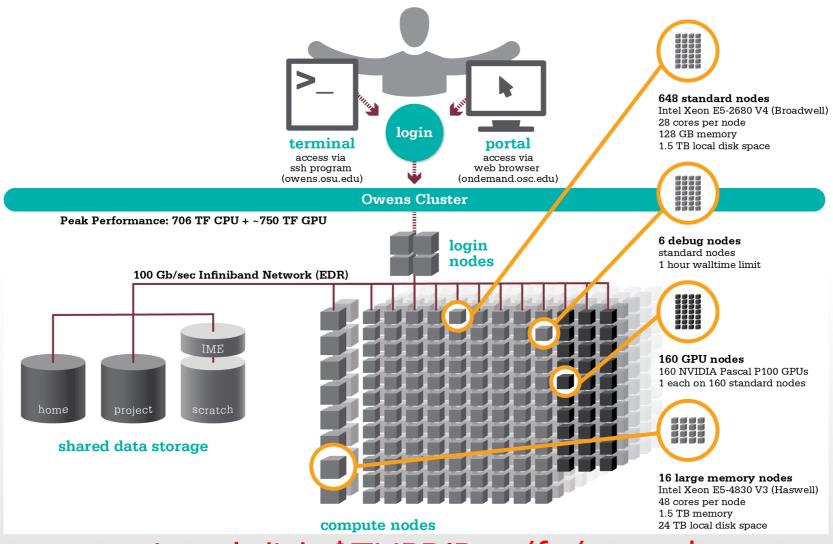
	Examples	Characteristics	Typical tools	Analytical methods
Small Data (megabytes)	Sales records, Customers database (small and medium companies)	Hundreds – thousands of records	Personal computer, Excel, R, other basic statistics software	Simple statistics
Large Data (gigabytes- terabytes)	Customer databases (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 Backed up daily Not backed up Permanent storage Temporary storage

Local disk: \$TMPDIR /fs/scratch: 1.5TB or 24TB

1200TB Not backed up 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

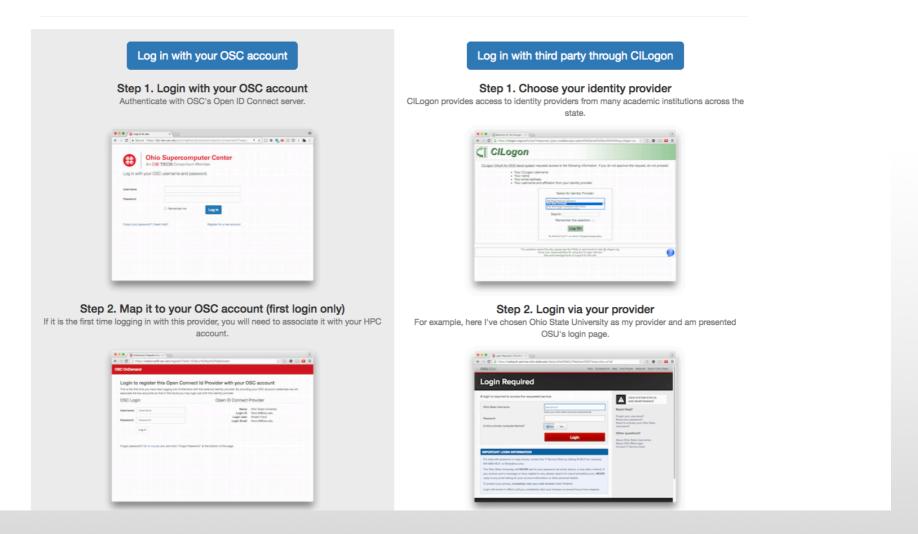


Go to https://ondemand.osc.edu/

OSC OnDemand

Login to OSC OnDemand

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





Ohio Supercomputer Center

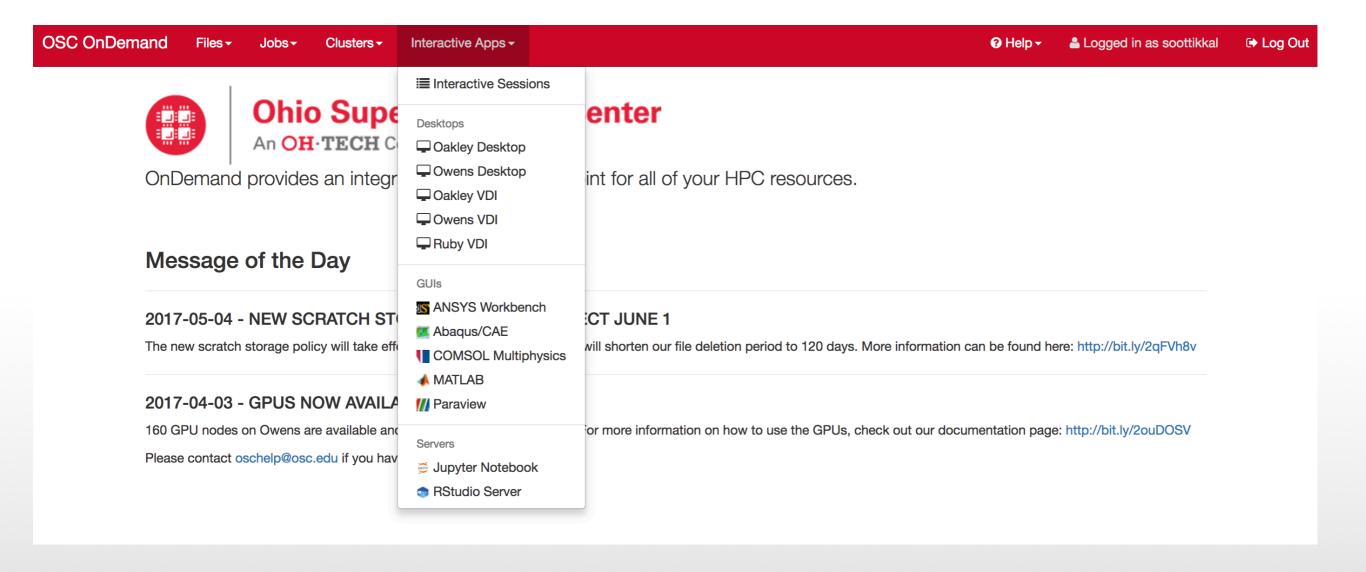
An **OH**·**TECH** Consortium Member

Log in with your OSC username and password.

Username	w687002	
Password	•••••	
	□ Remember me	Log in
Forgot your password?	Need Help? Register for a new account	











Exercise

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

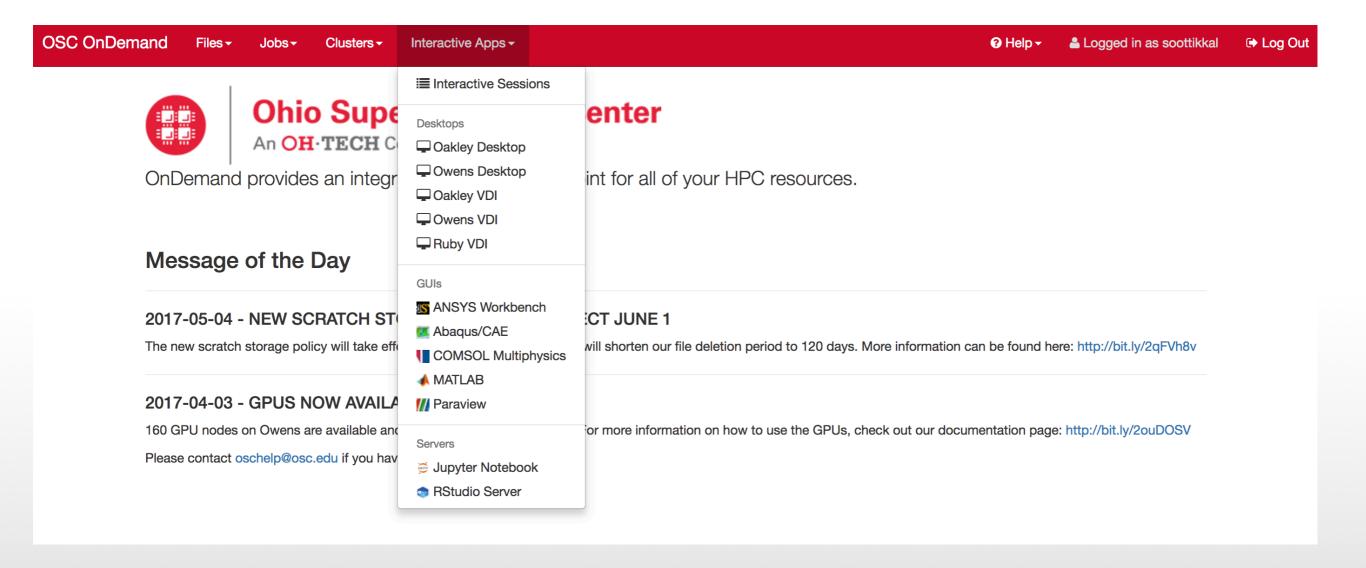
module load R
cd $PBS_O_WORKDIR
cp in.dat test.R $TMPDIR
cd $TMPDIR

R CMD BATCH test.R test.Rout

cp test.Rout $PBS_O_WORKDIR
```

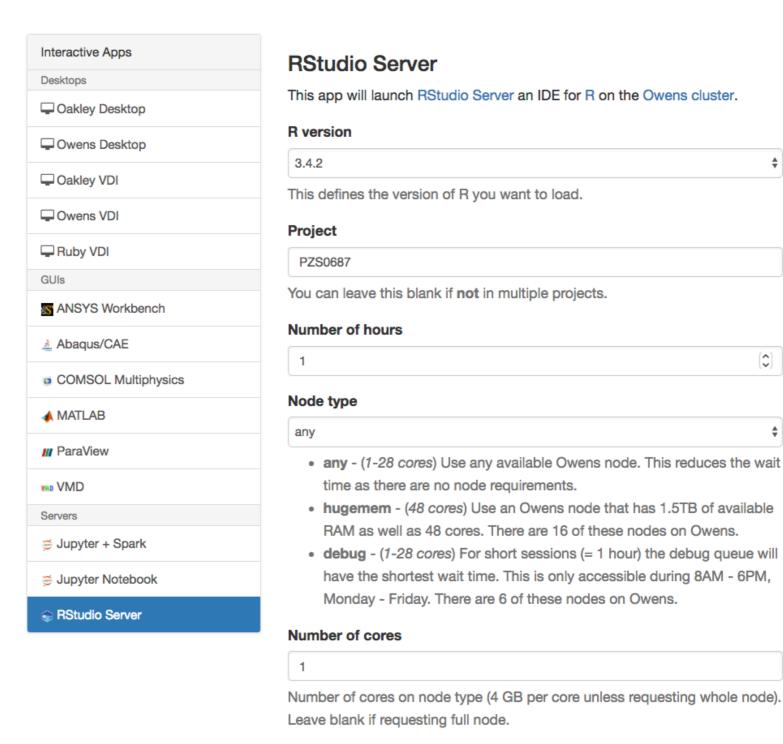


Rstudio on Ondemand







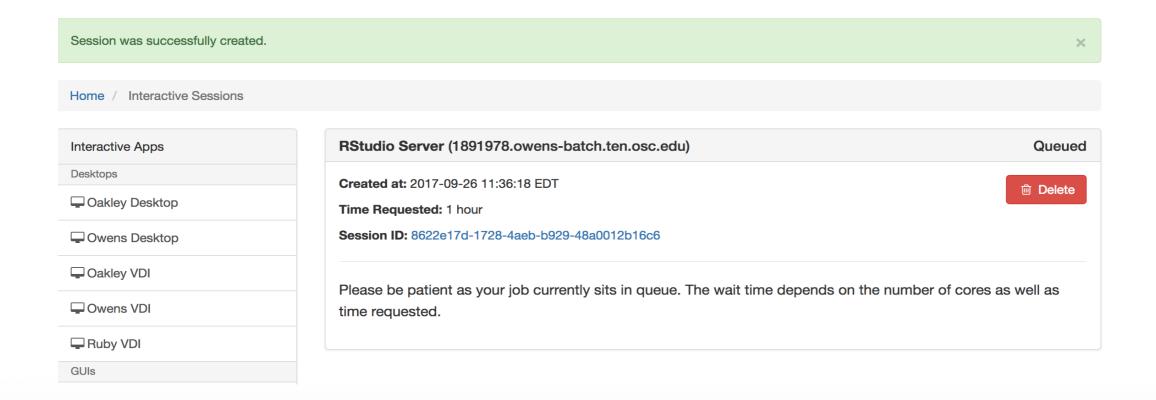


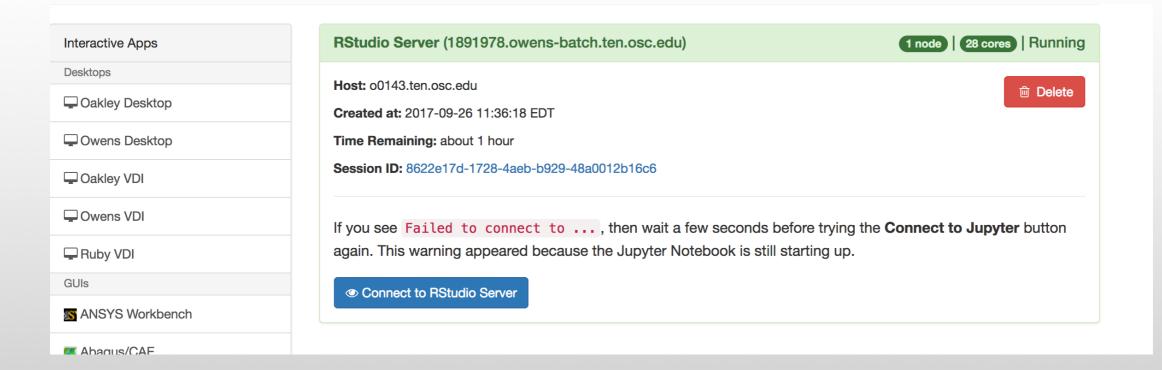
I would like to receive an email when the session starts

Launch



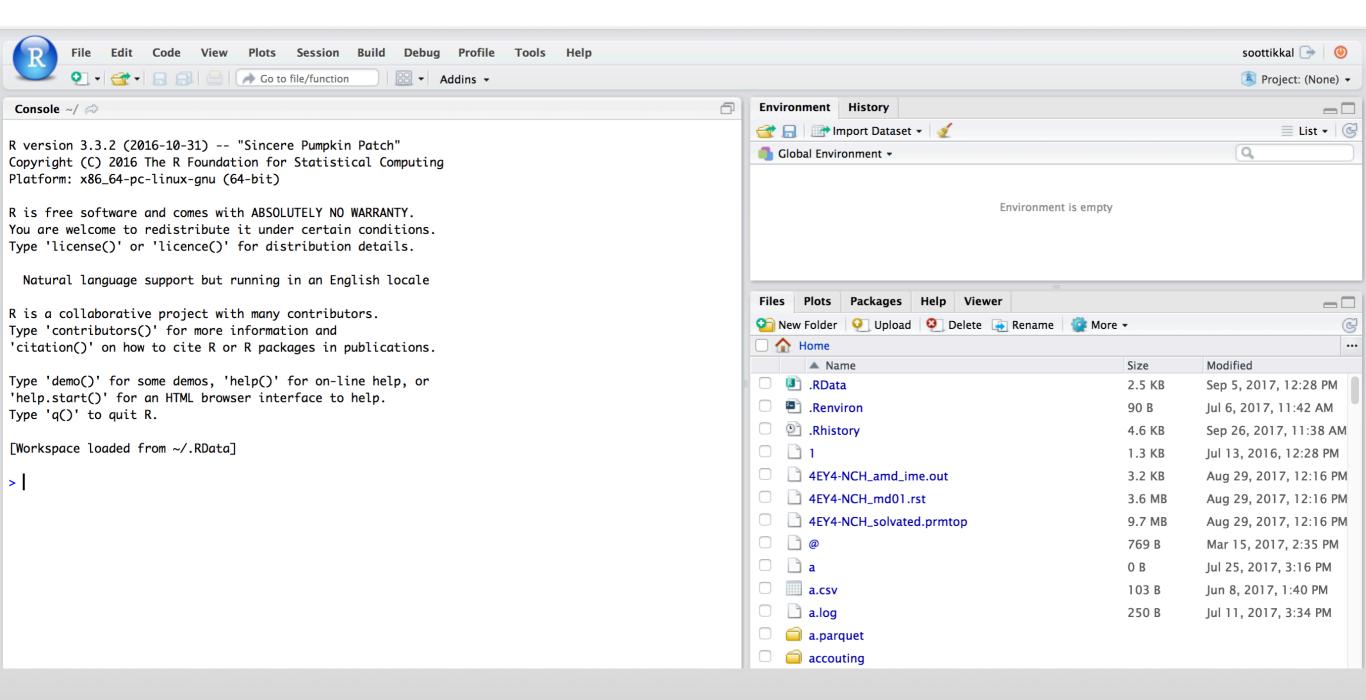




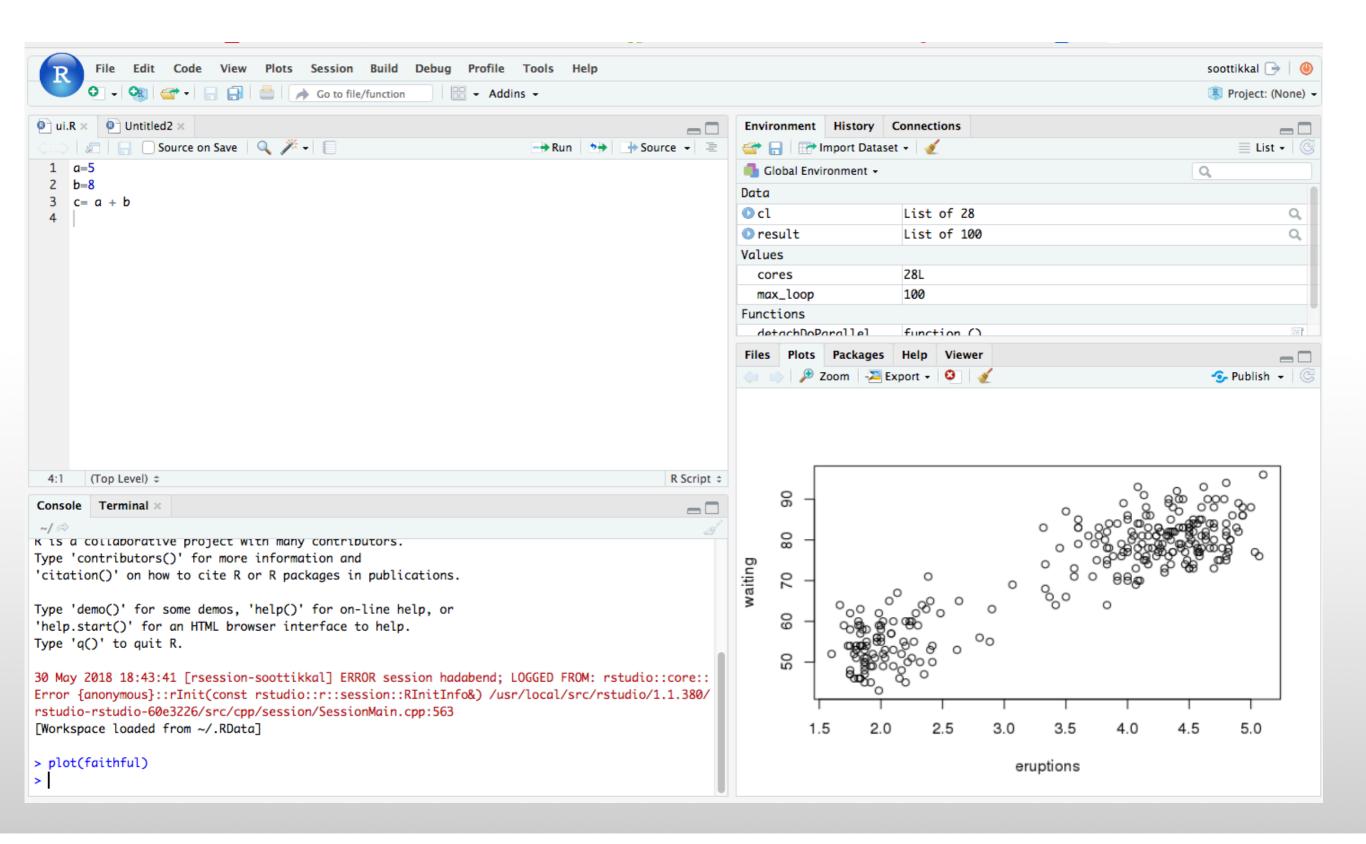














Exercise



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.

Ease of Use

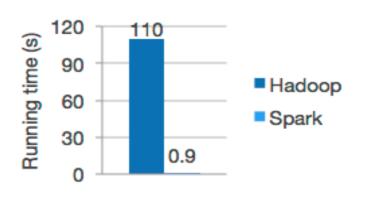
Write applications quickly in Java, Scala, Python, R.

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.

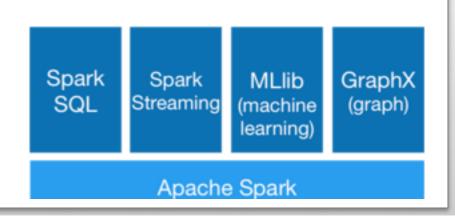
Generality

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.

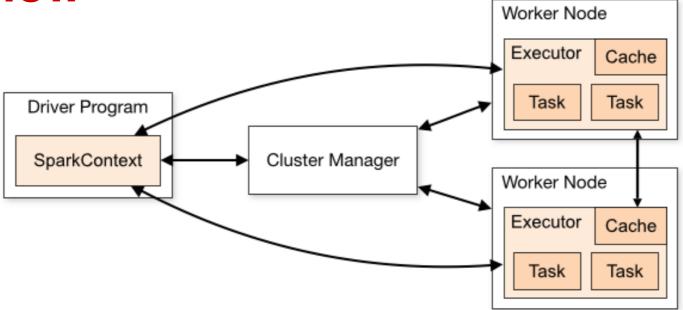


Logistic regression in Hadoop and Spark





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"?

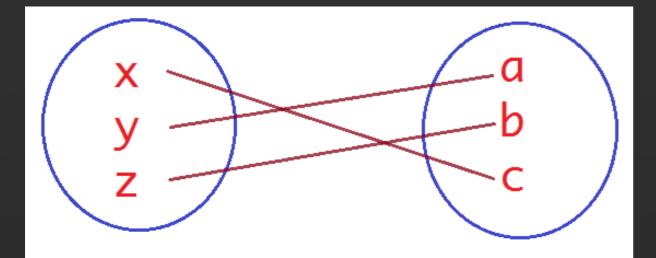


Word count Example

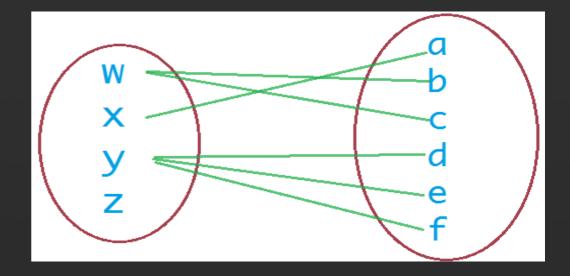
Map: One element in input gets mapped to only one element in output.

Flatmap: One element in input maps to zero or more elements in the output.

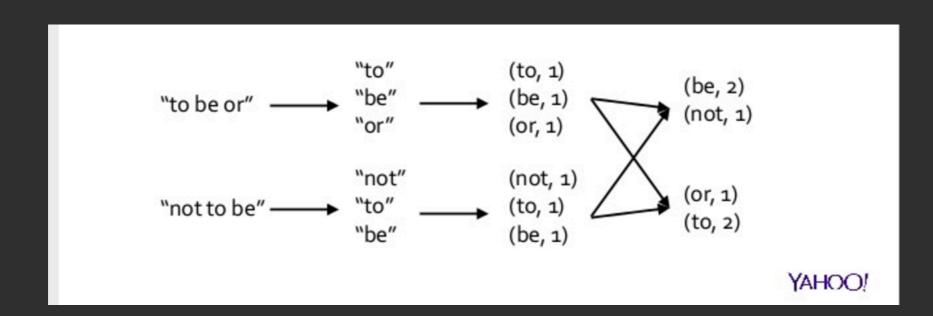
Мар



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



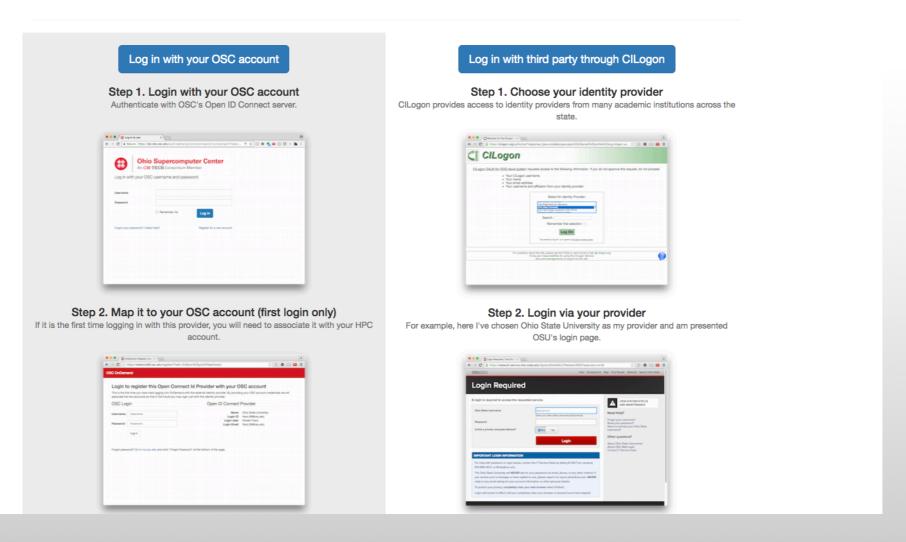
Running Spark interactively: Jupyter+Spark App

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

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Log in with your OSC username and password.

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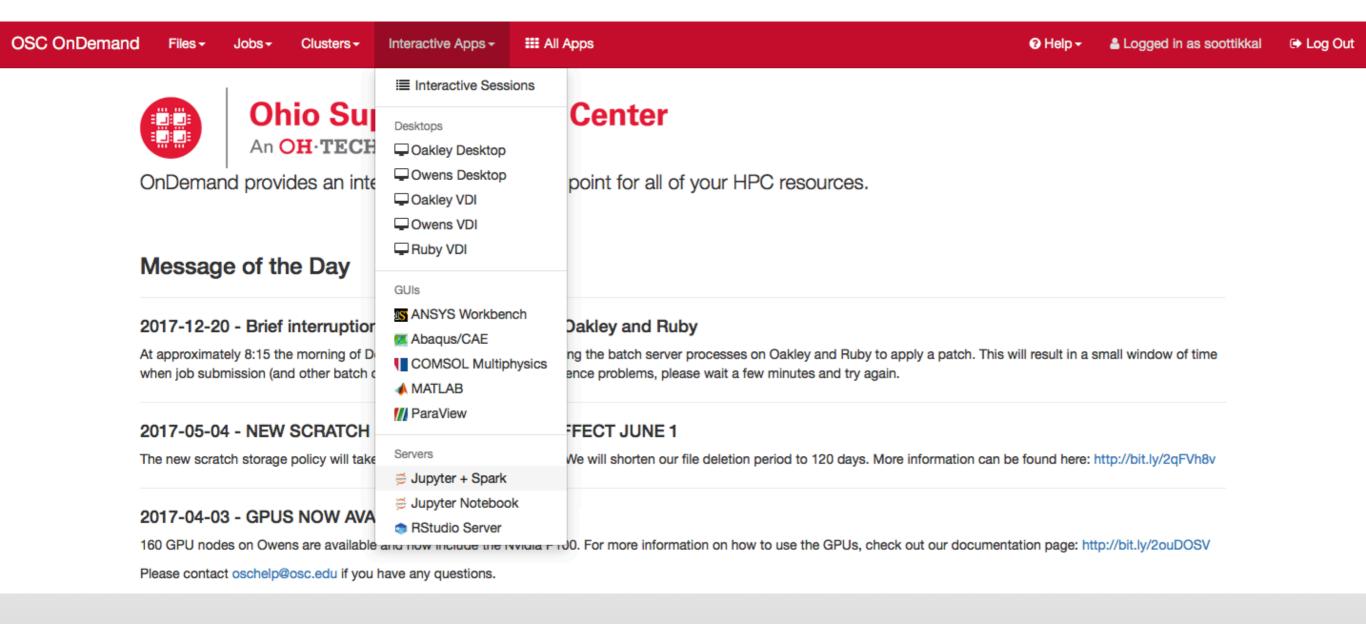
Log in with your OSC username and password.

Username	w687002	
Password	••••••	
	□ Remember me	Log in
Forgot your password?	Need Help? Register for a new account	





Choose Jupyter+Spark app from the Interactive Apps option.







OSC OnDernand Files → Jobs → Clusters → Interactive Apps → III My Interactive Sessions III All Apps

Home / My Interactive Sessions / Jupyter + Spark

Interactive Apps
Desktops
☐ Oakley Desktop
☐ Owens Desktop
☐ Oakley VDI
☐ Owens VDI
Ruby VDI
GUIs
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.

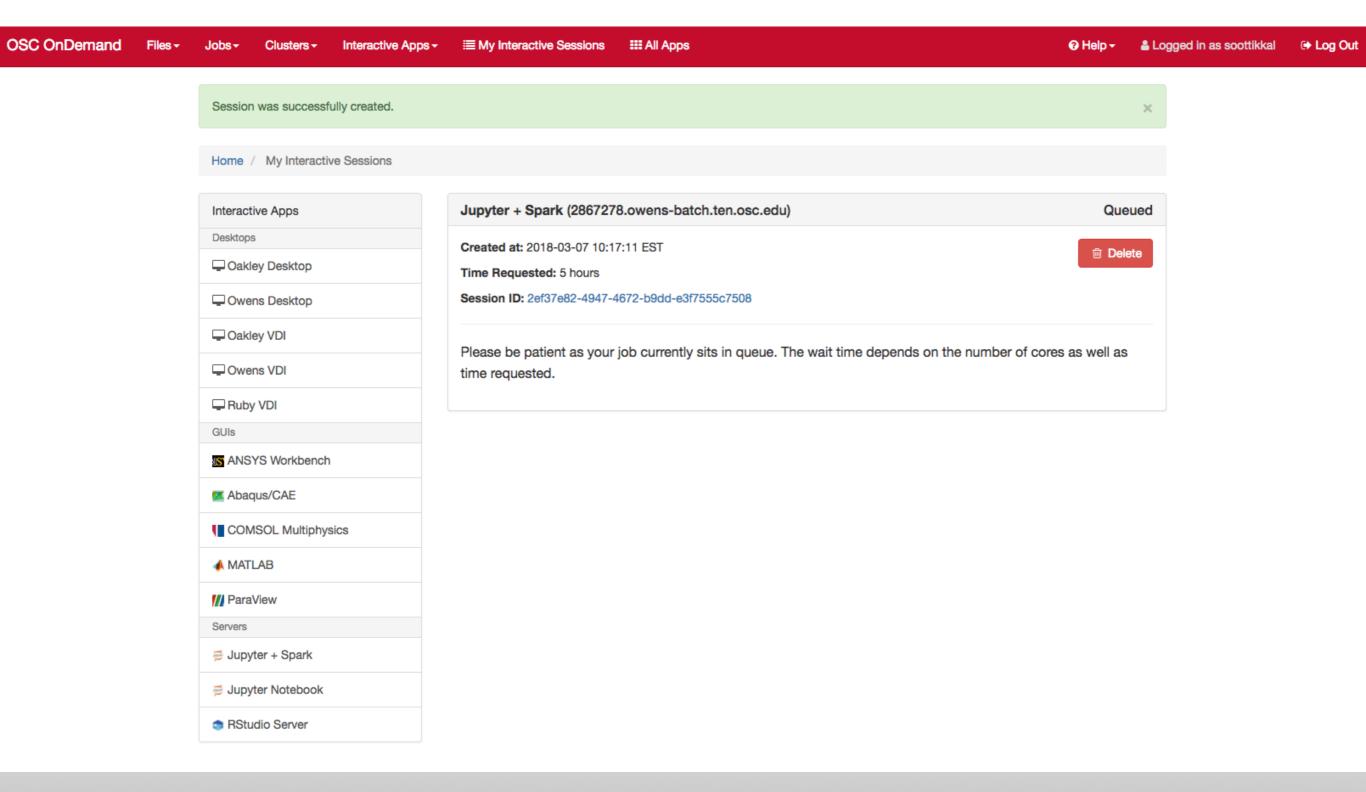
This is typically used for .collect and .take operations that require a large amount of memory allocated (> 2GB) for the driver process.

✓ Include access to OSC tutorial/workshop notebooks.

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

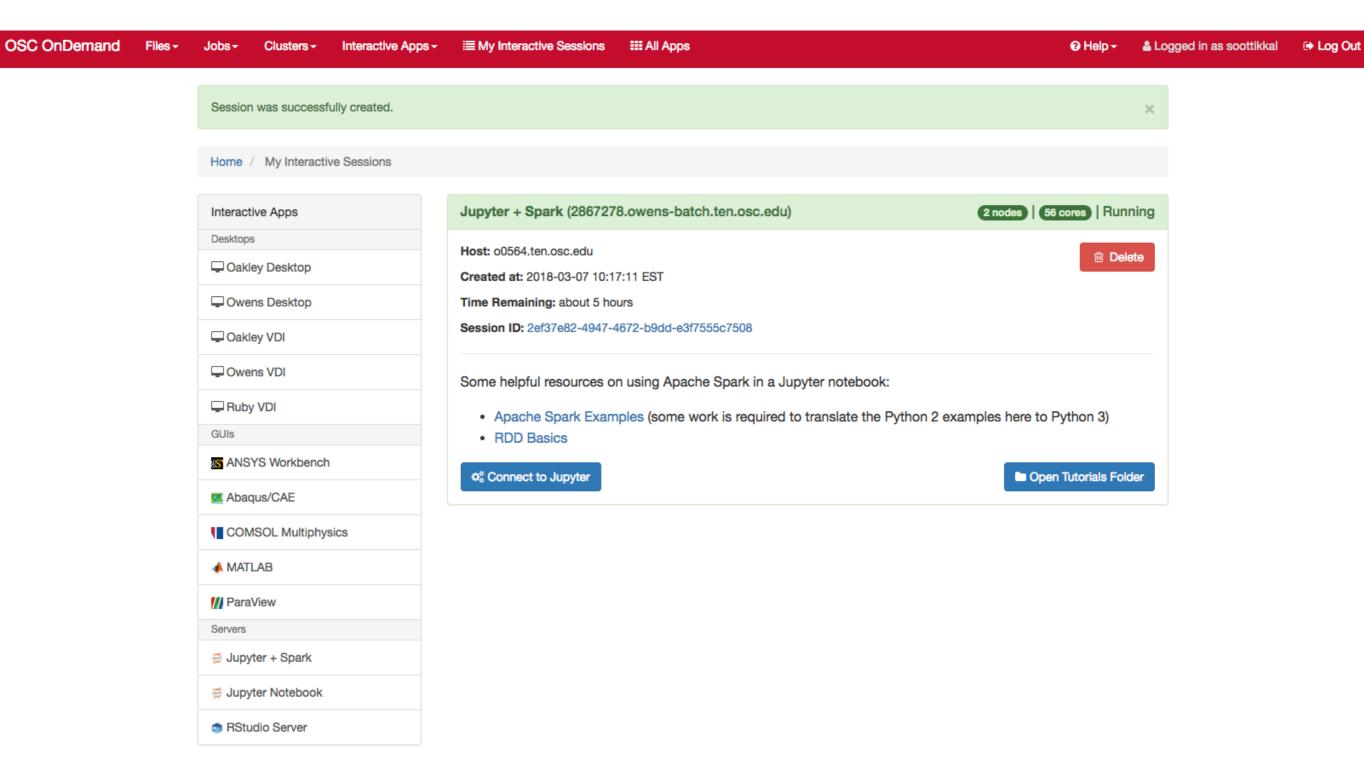
Launch

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











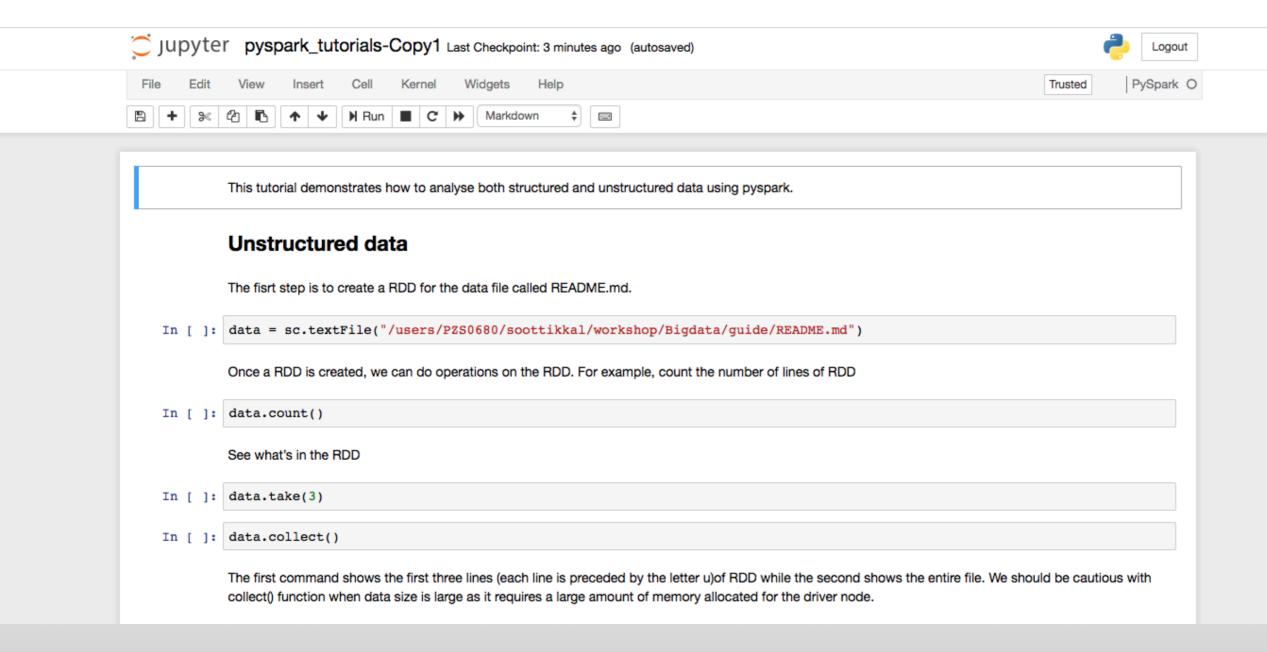


You will see a file called pyspark_tutorials.ipynb. Please check on the file and click on duplicate to make a copy of the file.



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.







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 fisrt 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



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
```

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 sqrt
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:/0//
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
```



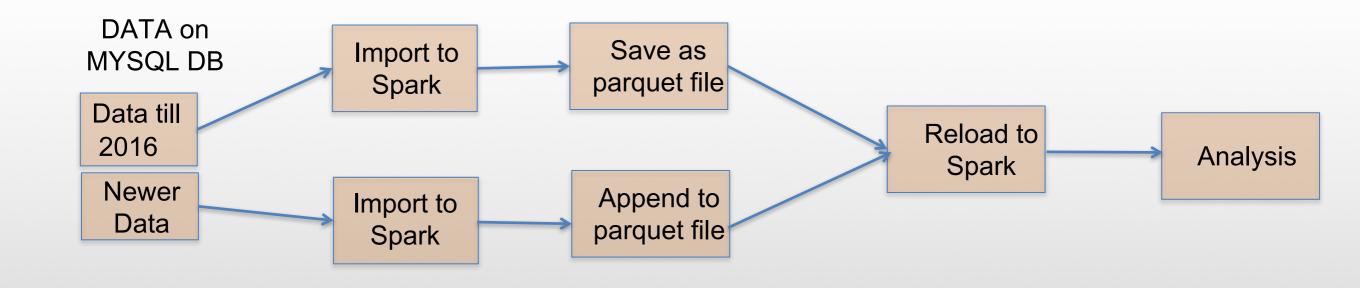
https://www.osc.edu/content/submitting_non_interactive_jobs

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|
13780.owens-batch...
                                         280| 2016-09-28|2016-10-08|MMPCDH24EC1-3-2eq...
13786.owens-batch...
                                        96 | 2016-09-28 | 2016-10-05 |
                             4 owens
                                                                               FR181-011DS|
                                                                                              foam|parallel
13798.owens-batch...
                                                                            TSRD-5-3-012DS1
                             30 | owens | 252 | 2016-09-28 | 2016-10-03 |
                                                                                              foam|parallel|
13800.owens-batch...
                             |0| owens|
                                         252 | 2016-09-28 | 2016-10-02 |
                                                                           TSRD-5-3-013MSE1
                                                                                              foam|parallel
                                         252 | 2016-09-28 | 2016-10-02 |
                                                                           TSRD-5-3-014MSE
13804.owens-batch...
                             10 | owens |
                                                                                              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()

.	
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|
```



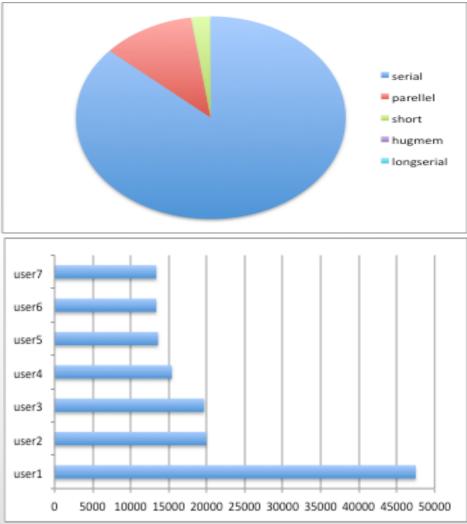
Results

Alien

Statistics			MYSQL		SPARK			
Job v	s CPU		1	hour		5	sec	
CPU vs Account		1.25 hour		5 sec				
Walltime vs		1.40 hour		5 sec				
user								
gromacs								
gaussian								
amber								
python								
qchem								
matlab								

1000000

1500000





500000

2000000

2500000

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)

Availability & Restrictions

Hadoop is available to all OSC users without restriction.

The following versions of Hadoop are available on OSC systems:

VERSION	OAKLEY	OWENS
3.0.0*		X

NOTE: * means it is the default version.

Set-up

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

module load hadoop

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

module load hadoop/3.0.0-alpha1

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
```



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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