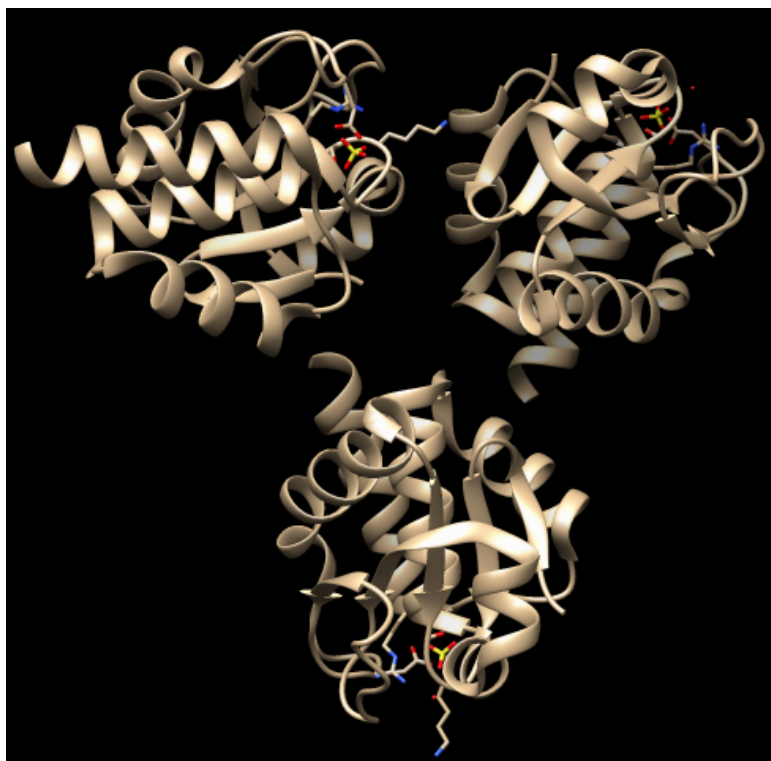# Multi-cloud Hadoop-based Dock Experiment

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Anthony Nguyen, UCSD, acn004@ucsd.edu
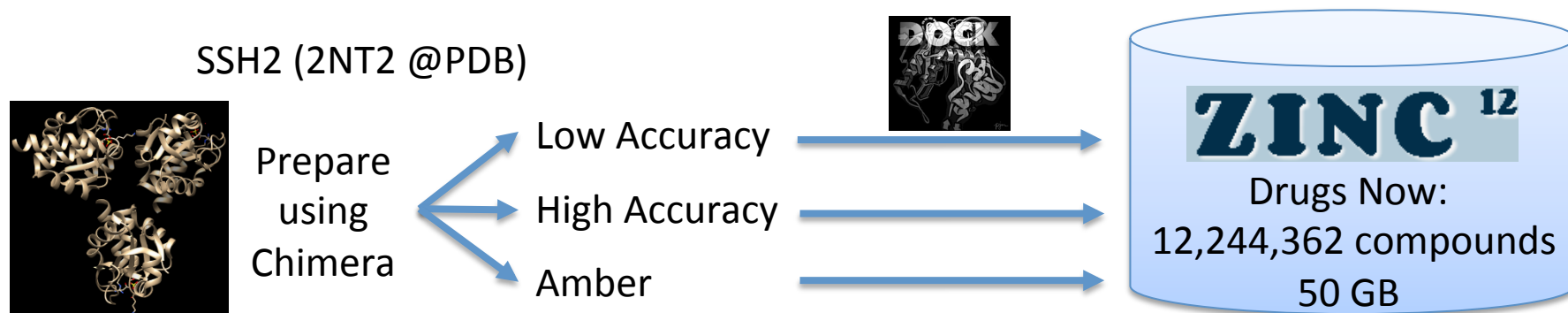Kohei Ichikawa, NAIST, ichikawa@is.naist.jp
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PRAGMA 28
April 10, 2015

National Institute of
Advanced Industrial Science
and Technology
AIST

NAIST
奈良先端科学技術大学院大学

UCSD

UF | UNIVERSITY of FLORIDA

Science: Dock

- Searches databases of ligands for compounds that bind a particular protein

SSH2 (2NT2 @PDB)

Prepare using Chimera

- Low Accuracy
- High Accuracy
- Amber

ZINC ^{12}

Drugs Now:
12,244,362 compounds
50 GB

	Time/mol	Time for ZINC	Time for ZINC on 100 cores	Time for 1% ZINC on 100 cores
Low Accuracy	10 sec	3.88 CPU-years	14.2 days	14.2 days
High Accuracy	6.6 min	153.7 CPU-years	1.53 years	5.58 days
Amber	30 min	698.9 CPU-years	6.98 years	25.47 days
		Total:	8.55 years	45.25 days
		Azure Price (D):	$1.3 million	$19,155
		Azure Price (G):	$1.9 million	$28,168

① Low Accuracy

② High Accuracy, Amber

Multi-Cloud Setup
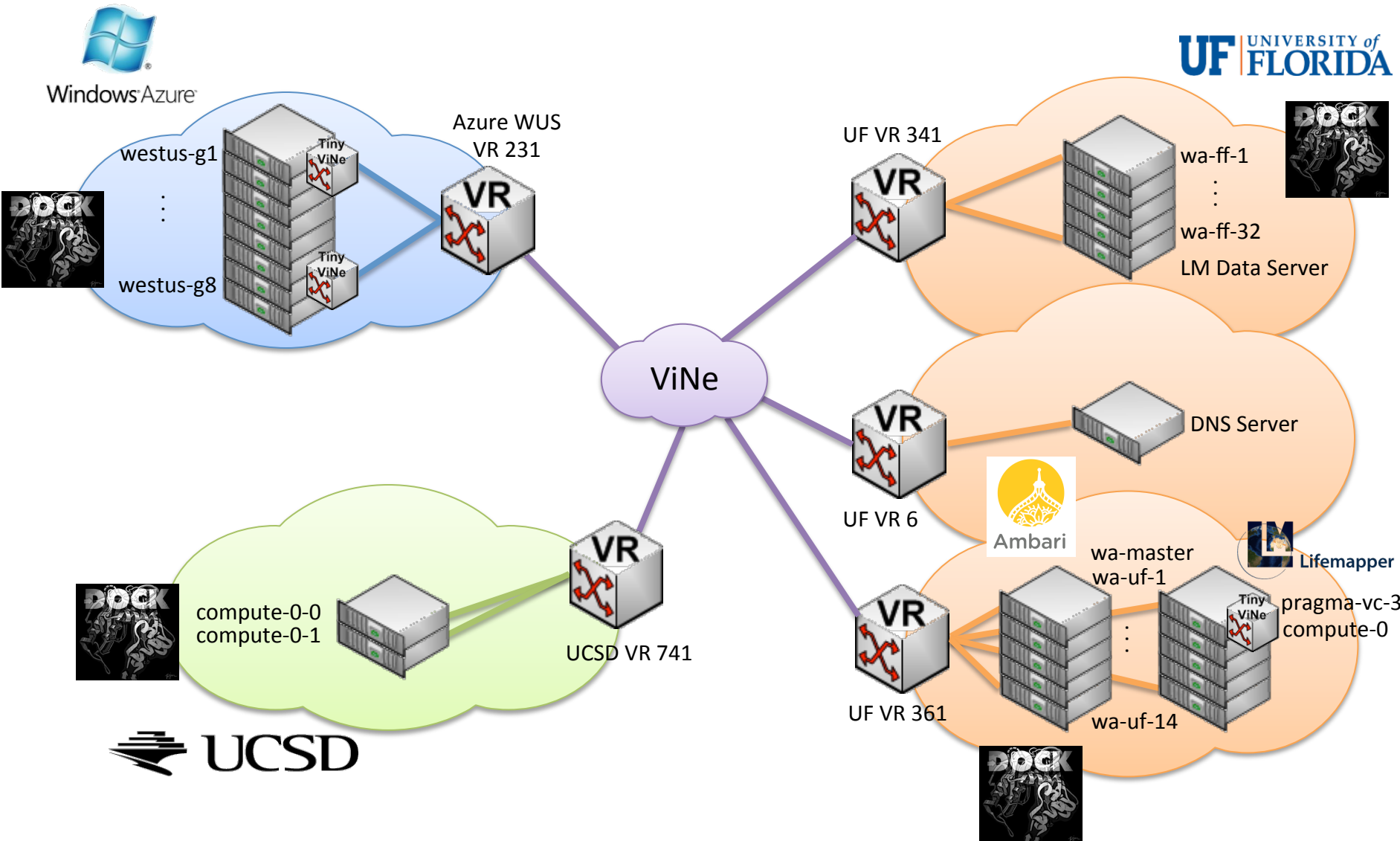
Dock on a Multi-Cloud

- Approach:
  - VM created on Azure contains Dock 6.2 compiled on 32-bit OS wrapped with UCSD fingerprinting tool to run on a 64-bit VM (make experiment reproducible)
  - VM converted to KVM image for UCSD and UF
  - Small modification to Dock source code to read molecule data through STDIN
  - Dock runs on Hadoop with streaming extension, and a pattern-based input splitter reused from CloudBLAST
  - Hadoop ecosystem deployed through Ambari
  - All VMs with all-to-all connectivity and DNS

Multi-Cloud Hadoop Motivation

- Take advantage of distributed pool of resources (private and public clouds)

- Have fault-tolerance during execution of dock

- Gain the ability to increase or decrease the number of resources used

- Reproducibility of experiment (by keeping consistency with previous environment and by having a homogeneous software stack)

- Make use of distributed storage

HDFS & Replication

- Replication factor: 3
- Fixed block size: 128 MB
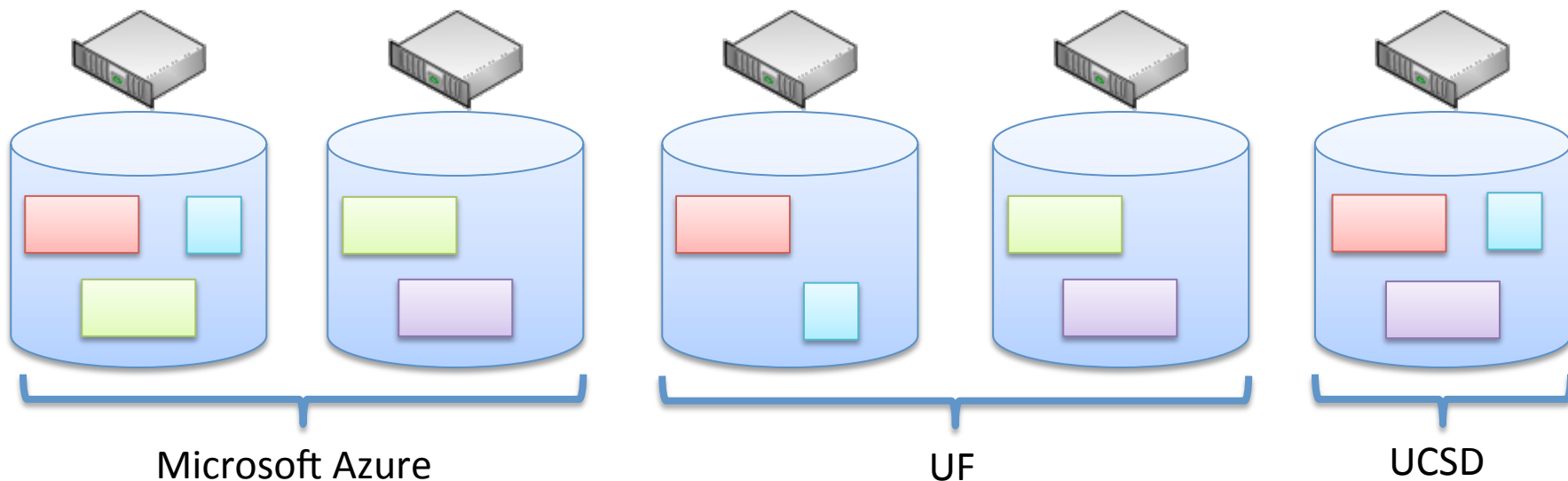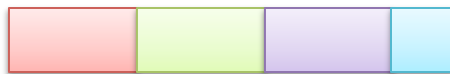
Ambari Dashboard

# Load on the Multi-Cloud Platform via Dashboard
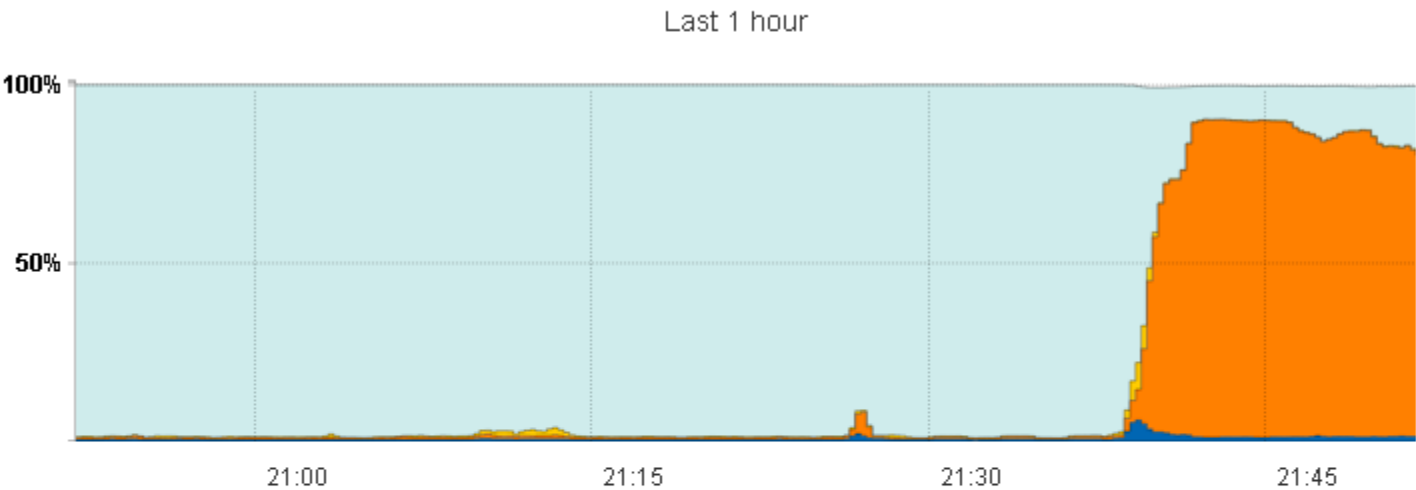
Load on the Multi-Cloud Platform via Ganglia

Stacked Graph - load_one

View Hosts

Add a Host

Add Host Wizard

Install Options

Enter the list of hosts to be included in the cluster and provide your SSH key.

Target Hosts

Enter a list of hosts using the Fully Qualified Domain Name (FQDN), one per line. Or use
Pattern Expressions

compute-0-1.local

Host Registration Information

⦿ Provide your SSH Private Key to automatically register hosts

Choose File   No file chosen

```
-----BEGIN RSA PRIVATE KEY-----
MIIEowIBAAKCAQEAvmF5rrX0hLpTG709ySIWQw0Z7K3caPZgHI4Xf1IR0rT
Yr9QV
```

SSH user (root or passwordless sudo account)   root

◯ Perform manual registration on hosts and do not use SSH

Register and Confirm →

Install Ambari Agent

PRAGYA

Add Host Wizard

Confirm Hosts

Registering your hosts.
Please confirm the host list and remove any hosts that you do not want to include in the cluster.

🗑 Remove Selected   Show: **All (1)** | Installing (1) | Registering (0) | Success (0) | Fail (0)

☐	Host	Progress	Status	Action
☐	compute-0-1.local		Installing	🗑 Remove

Show: 25 ▼   1 - 1 of 1   ⏮ ← → ⏭

← Back   Next →

Add Host as DataNode and NodeManager

Choose UCSD YARN Configuration Group

Add Host Wizard

ADD HOST WIZARD

Install Options

Confirm Hosts

Assign Slaves and Clients

Configurations

Review

Install, Start and Test

Summary

Configurations

Select the configuration groups to which the added hosts will belong to.

Service	Configuration Group
HDFS	HDFS Default ▾
YARN	UCSD ▾

← Back

Next →

Install Services on New Host

Browsing HDFS

HDFS Data Replication

HDFS Stores Output Replicated

Add Host Complete

Add Host Wizard

ADD HOST WIZARD

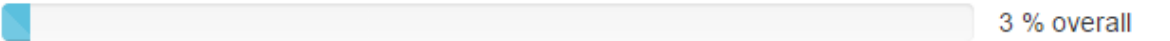Install Options
Confirm Hosts
Assign Slaves and Clients
Configurations
Review
Install, Start and Test
Summary

Install, Start and Test

Please wait while the selected services are installed and started.

100 % overall

Show: All (1) | In Progress (0) | Warning (0) | Success (1) | Fail (0)

Host	Status	Message
compute-0-1.local	100%	Success

1 of 1 hosts showing - Show All   Show: 25   1 - 1 of 1

Successfully installed and started the services.

Next →

Add Host Wizard

ADD HOST WIZARD

Install Options
Confirm Hosts
Assign Slaves and Clients
Configurations
Review
Install, Start and Test
Summary

Summary

Here is the summary of the install process.

The cluster consists of 25 hosts
   Installed and started services successfully on 1 new host
Install and start completed in 1 minutes and 21 seconds

Complete →

Computation Starts to Flow to New Host
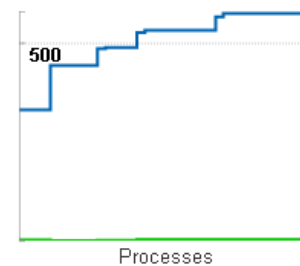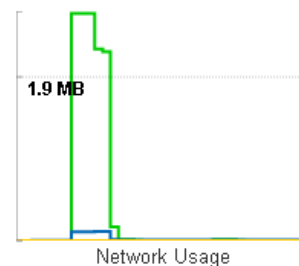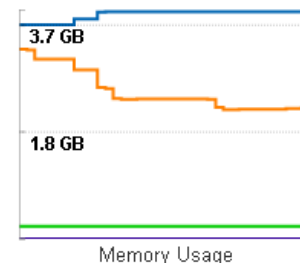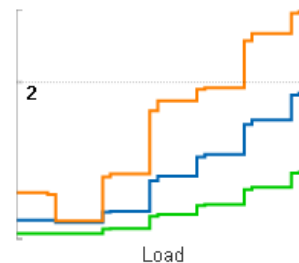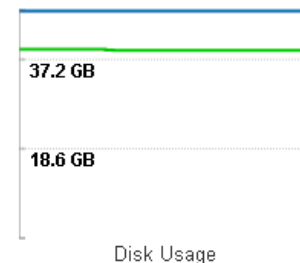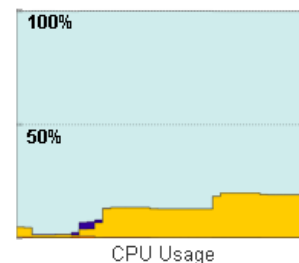
View Jobs and Its Completion Status

All Applications

Cluster
- About
- Nodes
- Applications
  - NEW
  - NEW_SAVING
  - SUBMITTED
  - ACCEPTED
  - RUNNING
  - FINISHED
  - FAILED
  - KILLED
- Scheduler

▸ Tools

Cluster Metrics

Apps Submitted	Apps Pending	Apps Running	Apps Completed	Containers Running	Memory Used	Memory Total	Memory Reserved	VCores Used	VCores Total	VCores Reserved	Active Nodes	Decommissioned Nodes	Lost Nodes	Unhealthy Nodes	Re
1	0	1	0	95	95 GB	104 GB	0 B	95	384	0	24	0	0	0	0

Show 20 entries   Search:

ID	User	Name	Application Type	Queue	StartTime	FinishTime	State	FinalStatus	Progress	Tracking
application_1428114831898_0001	mapred	streamjob2304626375912329697.jar	MAPREDUCE	default	Sat, 04 Apr 2015 03:05:15 GMT	N/A	RUNNING	UNDEFINED		Application

Showing 1 to 1 of 1 entries   First Previous 1 Next N

MapReduce Job
job_1428114831898_0001

▸ Cluster
▸ Application
▾ Job
- Overview
- Counters
- Configuration
- Map tasks
- Reduce tasks
- AM Logs

▸ Tools

Job Overview	
Job Name:	streamjob2304626375912329697.jar
State:	RUNNING
Uberized:	false
Started:	Sat Apr 04 03:05:06 UTC 2015
Elapsed:	9mins, 16sec

ApplicationMaster

Attempt Number	Start Time	Node	Logs
1	Sat Apr 04 03:04:59 UTC 2015	westus-g2.westus-g1.d1.internal.cloudapp.net:8042	logs

Task Type	Progress	Total	Pending	Running	Complete
Map		10000	9581	91	328
Reduce		0	0	0	0

Attempt Type	New	Running	Failed	Killed	Successful
Maps	9581	91	0	0	328
Reduces	0	0	0	0	0

View Map Execution Time

View and Control Services on Each Host
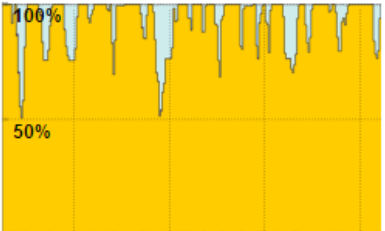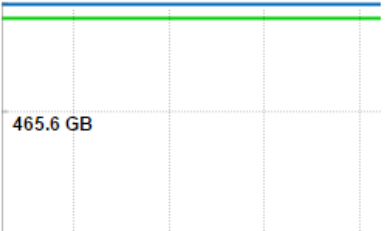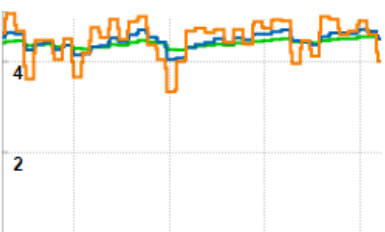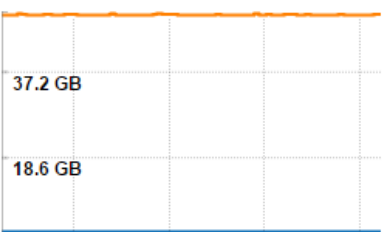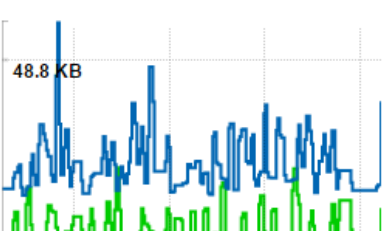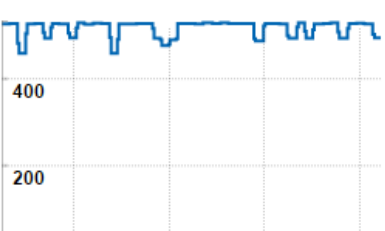
Lookup Service Usage via Heatmaps

Microsoft Azure Interface

Questions?

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Acknowledgements

Windows Azure

NSF

Thank you!