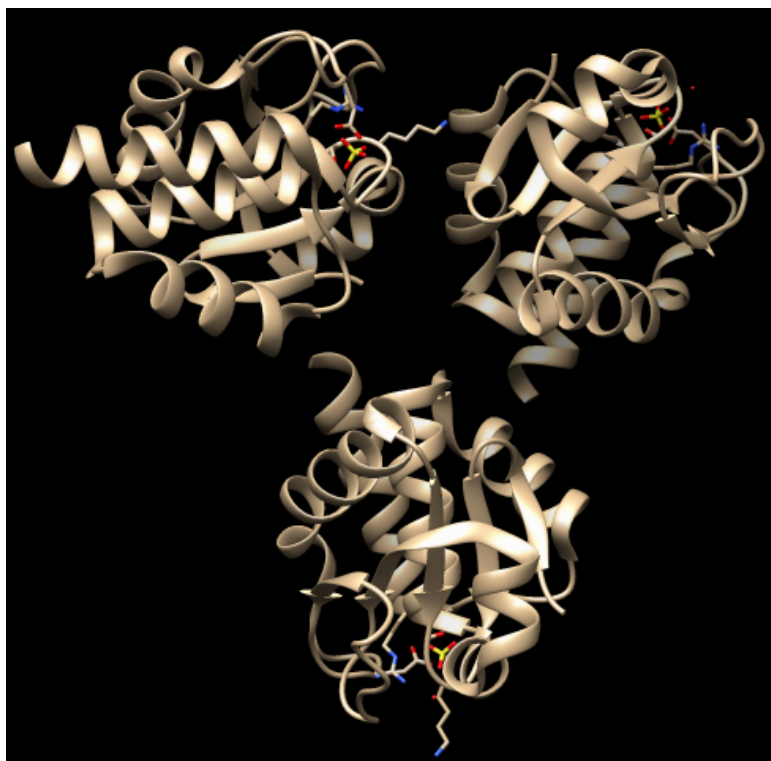


Multi-cloud Hadoop-based Dock Experiment



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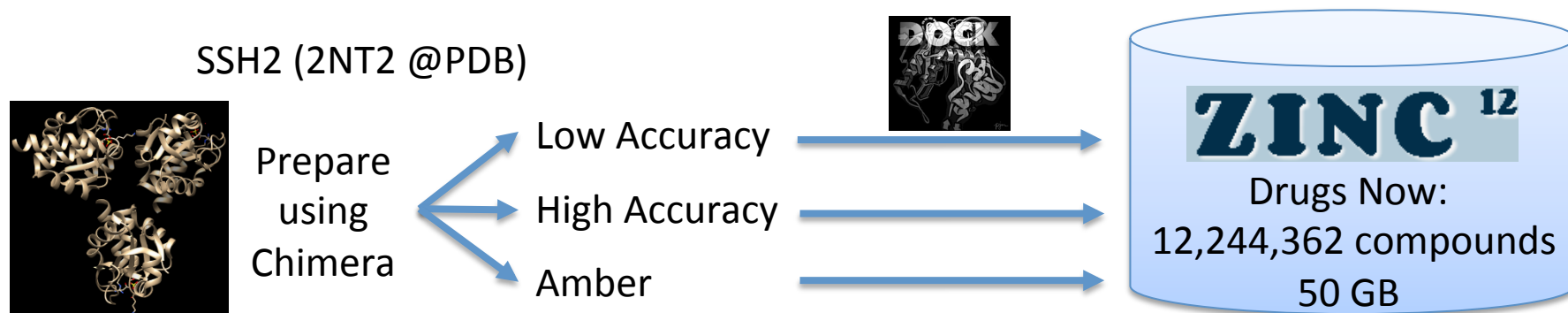
Jason Haga, AIST, jh.haga@aist.go.jp

PRAGMA 28

April 10, 2015

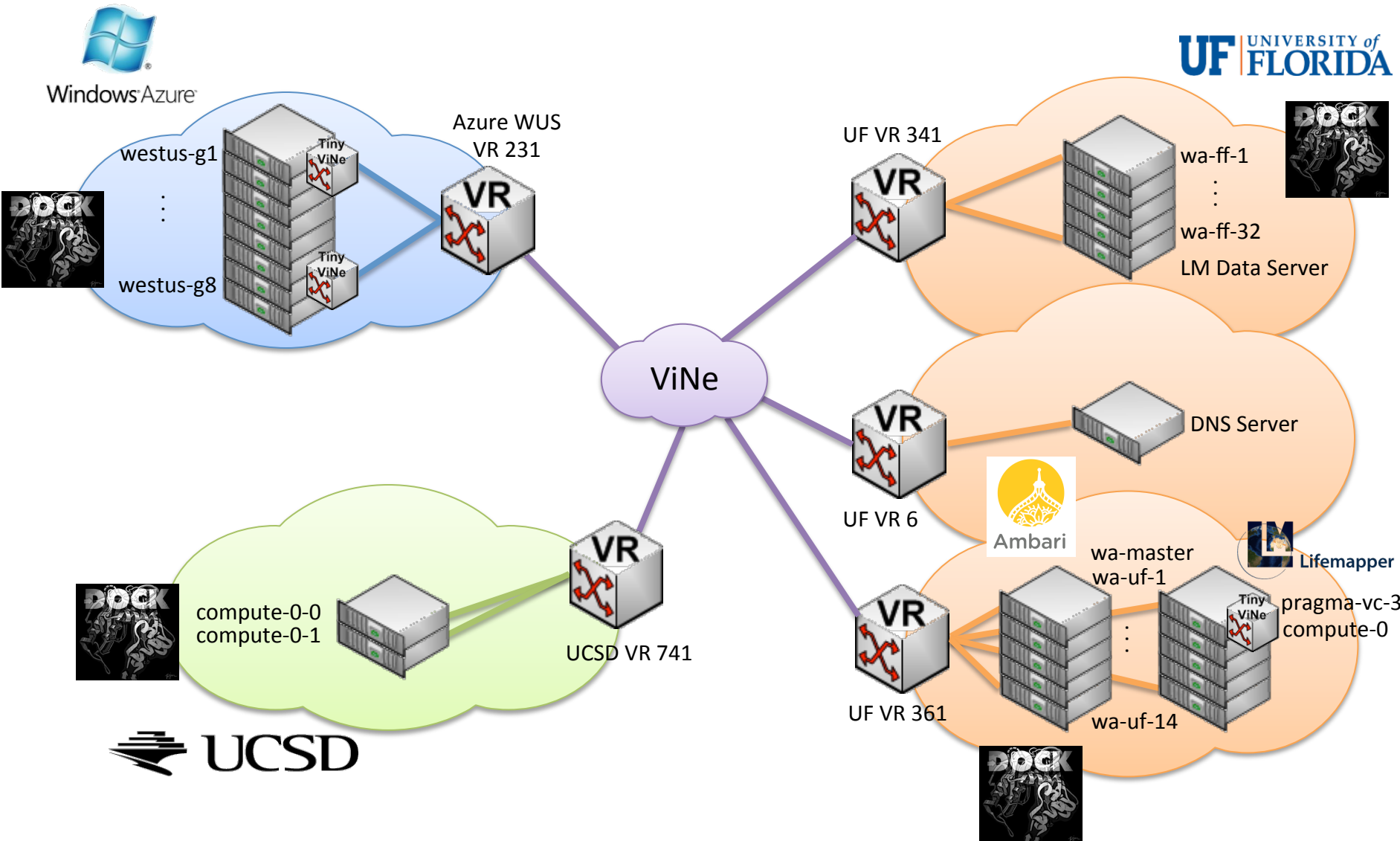
Science: Dock

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



		Time/mol	Time for ZINC	Time for ZINC on 100 cores	Time for 1% ZINC on 100 cores
①	Low Accuracy	10 sec	3.88 CPU-years	14.2 days	14.2 days
②	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

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

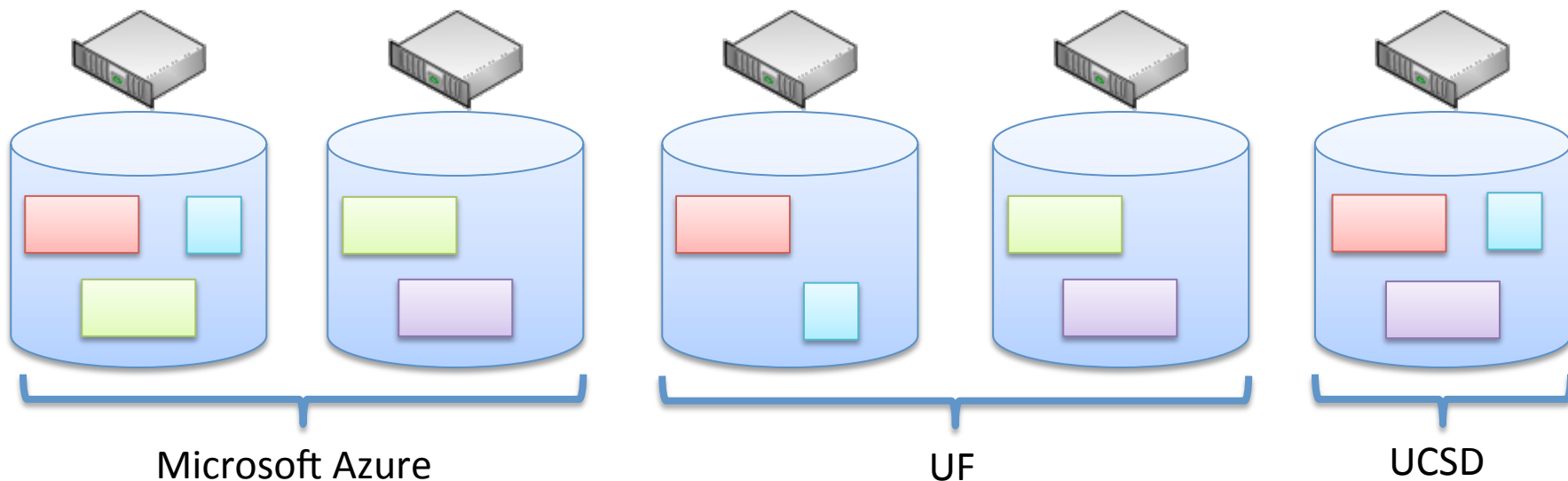
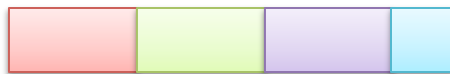
Multi-Cloud Hadoop Motivation

- 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

ZINC input file:



Ambari Dashboard

✓ HDFS

✓ MapReduce2

✓ YARN

✓ Ganglia

✓ ZooKeeper

Actions ▾

Metrics ▾

Heatmaps

Config History

HDFS Disk Usage

8%

DataNodes Live

23/23

HDFS Links

NameNode
Secondary NameNode
23 DataNodes

More... ▾

Memory Usage

465.6 GB

Network Usage

CPU Usage

100%

Cluster Load

100

NameNode Heap

6%

NameNode RPC

0.15 ms average RPC queue wait time

NameNode CPU WIO

0.6%

NameNode Uptime

1.9 d

ResourceManager Heap

6%

ResourceManager Uptime

1.9 d

NodeManagers Live

23/23

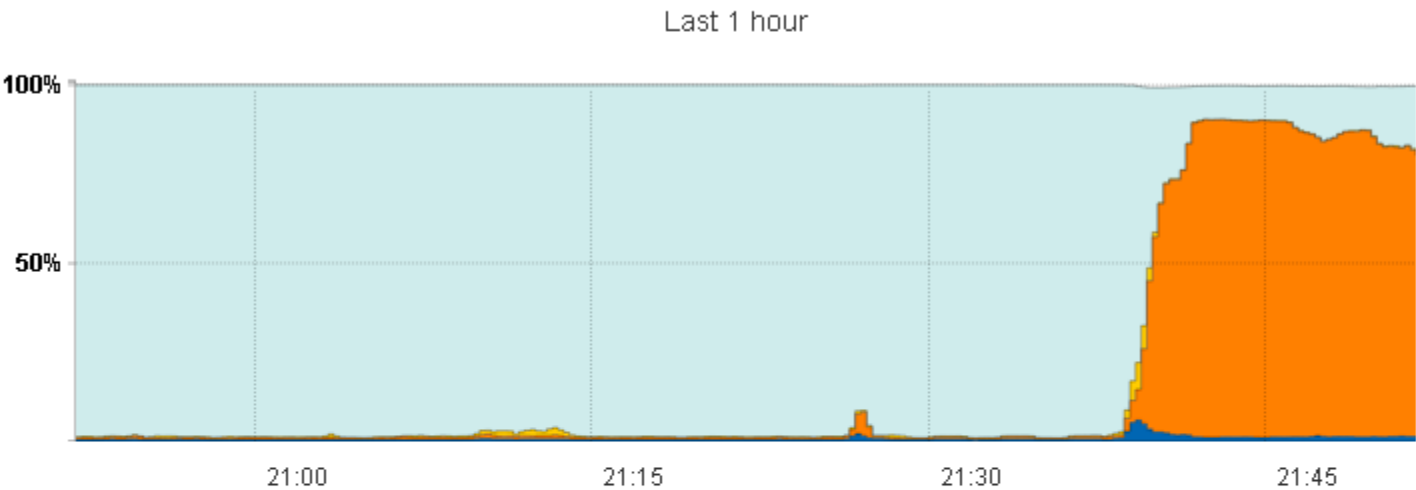
YARN Memory

95%

Load on the Multi-Cloud Platform via Dashboard

CPU Usage

X

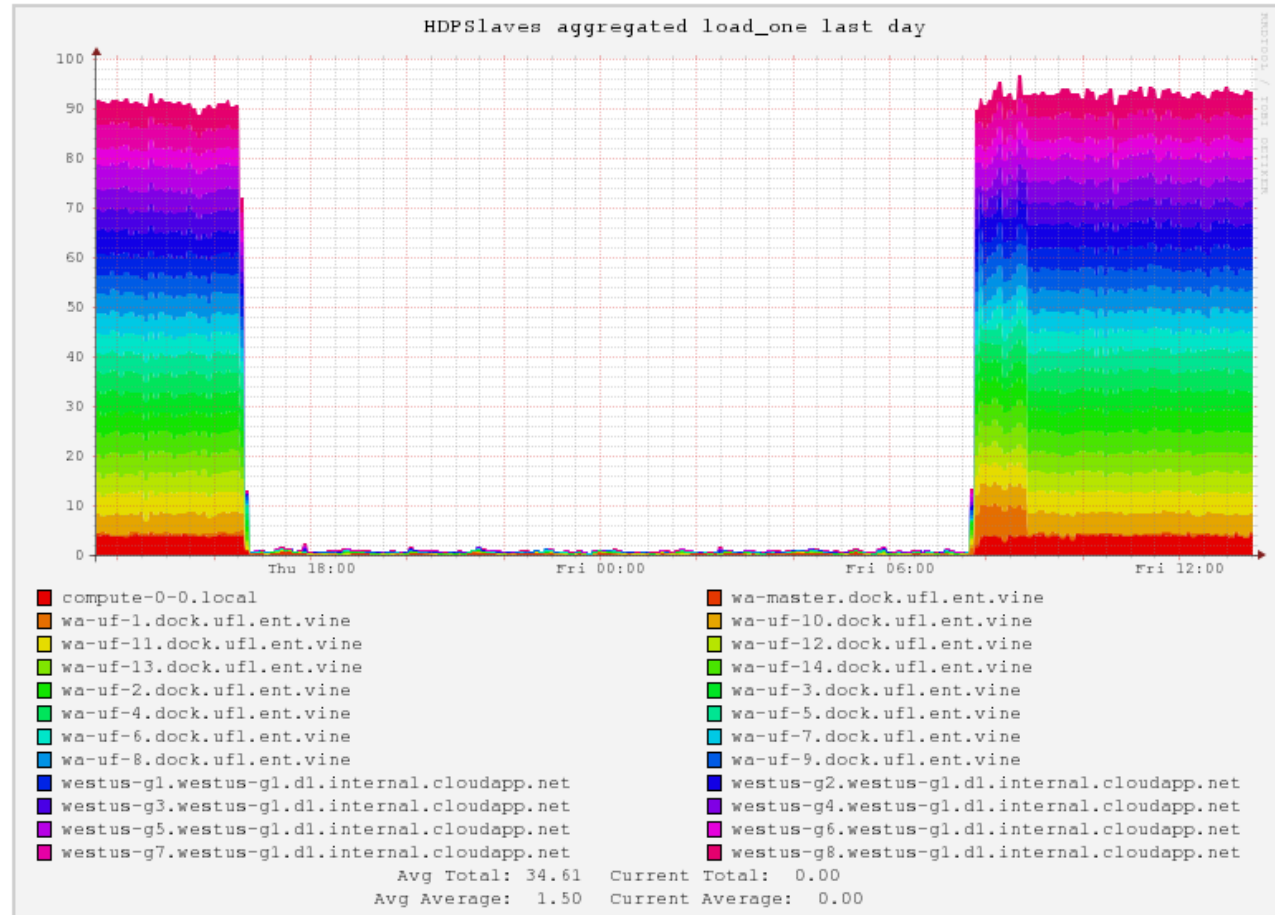


✓ Idle	min	9.382%	avg	81.114%	max	98.998%
✓ Wait	min	0.068%	avg	0.44%	max	7.527%
✓ User	min	0.294%	avg	17.499%	max	89.039%
✓ System	min	0.491%	avg	0.87%	max	5.969%
✓ Nice	min	0 %	avg	0 %	max	0%




















OK

Load on the Multi-Cloud Platform via Ganglia

Stacked Graph - load_one



View Hosts

Ambari pragma_dock 0 ops Dashboard Services Hosts Admin  admin							
Actions ▾		Filter: All (24) ▾					
Name	IP Address	Cores (CPU)	RAM	Disk Usage	Load Avg	Components	
<input type="checkbox"/> Any	<input type="text" value="Any"/>	<input type="text" value="Any"/>	<input type="text" value="Any"/>		<input type="text" value="Any"/>	<input type="button" value="Filter"/>	
<input type="checkbox"/>  compute-0-0.local	172.31.11.254	16 (16)	7.81GB	<div><div></div></div>	0.00	▶ 7 Components	
<input type="checkbox"/>  wa-master.dock.ufl.ent.vine	128.227.235.253	8 (8)	11.76GB	<div><div></div></div>	0.09	▶ 12 Components	
<input type="checkbox"/>  wa-uf-1.dock.ufl.ent.vine	172.24.59.41	4 (4)	5.84GB	<div><div></div></div>	0.08	▶ 3 Components	
<input type="checkbox"/>  wa-uf-10.dock.ufl.ent.vine	172.24.59.50	4 (4)	5.84GB	<div><div></div></div>	0.00	▶ 3 Components	
<input type="checkbox"/>  wa-uf-11.dock.ufl.ent.vine	172.24.59.51	4 (4)	5.84GB	<div><div></div></div>	0.05	▶ 3 Components	
<input type="checkbox"/>  wa-uf-12.dock.ufl.ent.vine	172.24.59.52	4 (4)	5.84GB	<div><div></div></div>	0.12	▶ 3 Components	
<input type="checkbox"/>  wa-uf-13.dock.ufl.ent.vine	172.24.59.53	4 (4)	5.84GB	<div><div></div></div>	0.01	▶ 3 Components	
<input type="checkbox"/>  wa-uf-14.dock.ufl.ent.vine	172.24.59.54	4 (4)	5.84GB	<div><div></div></div>	0.02	▶ 3 Components	
<input type="checkbox"/>  wa-uf-2.dock.ufl.ent.vine	172.24.59.42	4 (4)	5.84GB	<div><div></div></div>	0.00	▶ 3 Components	
<input type="checkbox"/>  wa-uf-3.dock.ufl.ent.vine	172.24.59.43	4 (4)	5.84GB	<div><div></div></div>	0.00	▶ 3 Components	
<input type="checkbox"/>  wa-uf-4.dock.ufl.ent.vine	172.24.59.44	4 (4)	5.84GB	<div><div></div></div>	0.00	▶ 3 Components	
<input type="checkbox"/>  wa-uf-5.dock.ufl.ent.vine	172.24.59.45	4 (4)	5.84GB	<div><div></div></div>	0.01	▶ 3 Components	
<input type="checkbox"/>  wa-uf-6.dock.ufl.ent.vine	172.24.59.46	4 (4)	5.84GB	<div><div></div></div>	0.01	▶ 3 Components	
<input type="checkbox"/>  wa-uf-7.dock.ufl.ent.vine	172.24.59.47	4 (4)	5.84GB	<div><div></div></div>	0.00	▶ 3 Components	
<input type="checkbox"/>  wa-uf-8.dock.ufl.ent.vine	172.24.59.48	4 (4)	5.84GB	<div><div></div></div>	0.01	▶ 3 Components	
<input type="checkbox"/>  wa-uf-9.dock.ufl.ent.vine	172.24.59.49	4 (4)	5.84GB	<div><div></div></div>	0.04	▶ 3 Components	
<input type="checkbox"/>  westus-g1.westus-g1.d1.inter...	172.24.60.5	4 (4)	55.15GB	<div><div></div></div>	0.00	▶ 7 Components	
<input type="checkbox"/>  westus-g2.westus-g1.d1.inter...	172.24.60.6	4 (4)	55.15GB	<div><div></div></div>	0.00	▶ 3 Components	

Add a Host

Add Host Wizard

X

ADD HOST WIZARD

Install Options

[Confirm Hosts](#)[Assign Slaves and Clients](#)[Configurations](#)[Review](#)[Install, Start and Test](#)[Summary](#)

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)

- ☐ Perform [manual registration](#) on hosts and do not use SSH

Register and Confirm →

Install Ambari Agent

Add Host Wizard

ADD HOST WIZARD

[Install Options](#)

Confirm Hosts

[Assign Slaves and Clients](#)

[Configurations](#)

[Review](#)

[Install, Start and Test](#)

[Summary](#)

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 \(0\)](#)

<input type="checkbox"/>	Host	Progress	Status	Action
<input type="checkbox"/>	compute-0-1.local	<div></div>	Installing	<div>Remove</div>

Show: 25

1 - 1 of 1

⏮

⏪

⏩

⏭

Add Host as DataNode and NodeManager

Add Host Wizard

ADD HOST WIZARD

[Install Options](#)[Confirm Hosts](#)**Assign Slaves and Clients**[Configurations](#)[Review](#)[Install, Start and Test](#)[Summary](#)

Assign Slaves and Clients

Assign slave and client components to hosts you want to run them on.

Hosts that are assigned master components are shown with ✱.

"Client" will install HDFS Client, MapReduce2 Client, YARN Client and ZooKeeper Client.

Host	all none	all none	all none
compute-0-1.local	<input checked="" type="checkbox"/> DataNode	<input checked="" type="checkbox"/> NodeManager	<input type="checkbox"/> Client

Show: 25 ▼

1 - 1 of 1

⏮ ⏪ ⏩ ⏭

[← Back](#)[Next →](#)

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

Add Host Wizard

ADD HOST WIZARD

Install Options

Confirm Hosts

Assign Slaves and Clients

Configurations

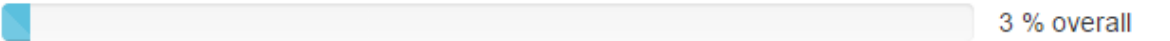
Review

Install, Start and Test

Summary

Install, Start and Test

Please wait while the selected services are installed and started.



Show: **All (1)** | [In Progress \(1\)](#) | [Warning \(0\)](#) | [Success \(0\)](#) | [Fail \(0\)](#)

Host	Status	Message
compute-0-1.local	<div></div> 3%	Waiting to install DataNode

1 of 1 hosts showing - [Show All](#) Show: 25 ▼ 1 - 1 of 1 ⏮ ⏪ ⏩ ⏭

Next →

Browsing HDFS

[Hadoop](#)[Overview](#)[Datanodes](#)[Snapshot](#)[Startup Progress](#)[Utilities](#)

Browse Directory

Go!

Permission	Owner	Group	Size	Replication	Block Size	Name
-rw-r--r--	mapred	hdfs	572.21 MB	3	128 MB	23_p0.1.mol2
-rw-r--r--	mapred	hdfs	572.21 MB	3	128 MB	23_p0.4.mol2

HDFS Data Replication

File information - 23_p0.1.mol2

File information - 23_p0.1.mol2

×

[Download](#)

[Download](#)

Block information -- Block 0 ▾

Block ID: 1073751880

Block Pool ID: BP-459779146-172.24.59.240-1427918995831

Generation Stamp: 11056

Size: 134217728

Availability:

- westus-g6.westus-g1.d1.internal.cloudapp.net
- wa-uf-10.dock.ufl.ent.vine
- wa-uf-9.dock.ufl.ent.vine

Block information -- Block 1 ▾

Block ID: 1073751881

Block Pool ID: BP-459779146-172.24.59.240-1427918995831

Generation Stamp: 11057

Size: 134217728

Availability:

- wa-uf-2.dock.ufl.ent.vine
- wa-uf-14.dock.ufl.ent.vine
- westus-g5.westus-g1.d1.internal.cloudapp.net

3 Replicas

Close

HDFS Stores Output Replicated

Hadoop

Overview

Datanodes

Snapshot

Startup Progress

Utilities ▾

Browse Directory

File information - part-00000



/mapred/output/23_p0.1_dc

Download

Go!

Permission	O
-rw-r--r--	m
-rw-r--r--	m
-rw-r--r--	m
-rw-r--r--	m
-rw-r--r--	m
-rw-r--r--	m
-rw-r--r--	m
-rw-r--r--	m
-rw-r--r--	m

Block information -- Block 0 ▾

Block ID: 1073752115

Block Pool ID: BP-459779146-172.24.59.240-1427918995831

Generation Stamp: 11291

Size: 11814

Availability:

- wa-uf-9.dock.ufl.ent.vine
- westus-g7.westus-g1.d1.internal.cloudapp.net
- westus-g3.westus-g1.d1.internal.cloudapp.net

Name
_SUCCESS
part-00000
part-00001
part-00002
part-00003
part-00004
part-00005
part-00006
part-00007

Close

Add Host Complete

Add Host Wizard

X

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.



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

Host	Status	Message
compute-0-1.local	<div></div> 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

X

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

✓ **compute-0-1.local** No alerts

← Back

Summary

Configs

Host Actions ▾

Components

+ Add

✓ DataNode / [HDFS](#)

Started ▾

✓ Ganglia Monitor / [Ganglia](#)

Started ▾

✓ NodeManager / [YARN](#)

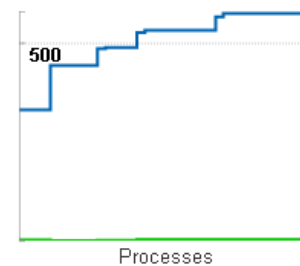
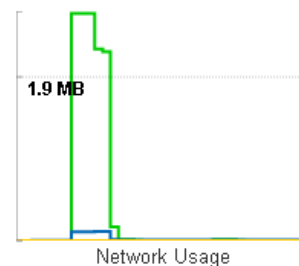
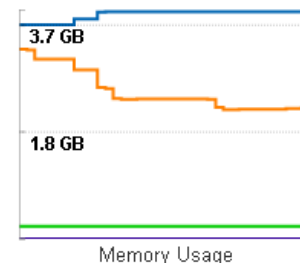
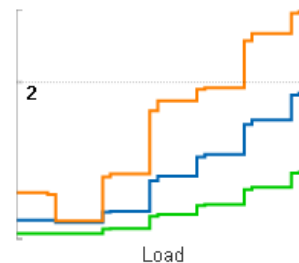
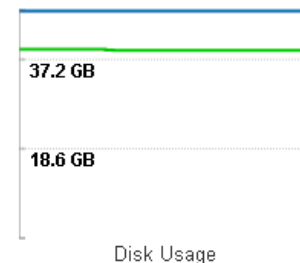
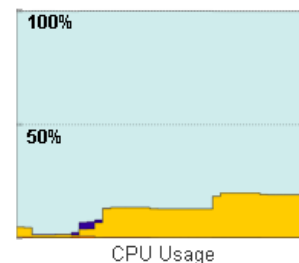
Started ▾

Summary

Hostname: compute-0-1.local
IP Address: 172.31.11.253
OS: centos6 (x86_64)
Cores (CPU): 16 (16)
Disk: 8.19GB/47.36GB (17.28% used)
Memory: 7.81GB
Load Avg: 2.90
Heartbeat: a moment ago

Host Metrics

🔗



View Jobs and Its Completion Status



Logged in as

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



Logged in as: dr.who

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

Logged in as: dr.who



Map Tasks for job_1428114831898_0001

- ▶ Cluster
- ▶ Application
- ▼ Job
 - [Overview](#)
 - [Counters](#)
 - [Configuration](#)
 - [Map tasks](#)
 - [Reduce tasks](#)
 - [AM Logs](#)
- ▶ Tools

Show 20 entries Search: <input type="text"/>						
Task ^	Progress ↕	Status ↕	State ↕	Start Time ↕	Finish Time ↕	Elapsed Time ↕
task_1428114831898_0001_m_000000	<div></div>	Records R/W=27/471	SUCCEEDED	Sat, 04 Apr 2015 03:05:11 GMT	Sat, 04 Apr 2015 03:13:22 GMT	8mins, 11sec
task_1428114831898_0001_m_007419	<div></div>	Records R/W=5/185	SUCCEEDED	Sat, 04 Apr 2015 03:14:34 GMT	Sat, 04 Apr 2015 03:15:50 GMT	1mins, 16sec
task_1428114831898_0001_m_000002	<div></div>	Records R/W=25/428	SUCCEEDED	Sat, 04 Apr 2015 03:05:11 GMT	Sat, 04 Apr 2015 03:12:22 GMT	7mins, 10sec
task_1428114831898_0001_m_000003	<div></div>	Records R/W=24/432	SUCCEEDED	Sat, 04 Apr 2015 03:05:11 GMT	Sat, 04 Apr 2015 03:12:50 GMT	7mins, 39sec
task_1428114831898_0001_m_000004	<div></div>	Records R/W=21/1	SUCCEEDED	Sat, 04 Apr 2015 03:05:12 GMT	Sat, 04 Apr 2015 03:06:15 GMT	1mins, 3sec
task_1428114831898_0001_m_000005	<div></div>	Records R/W=25/1	SUCCEEDED	Sat, 04 Apr 2015 03:05:12 GMT	Sat, 04 Apr 2015 03:06:13 GMT	1mins, 1sec
task_1428114831898_0001_m_000006	<div></div>	Records R/W=22/1	SUCCEEDED	Sat, 04 Apr 2015 03:05:12 GMT	Sat, 04 Apr 2015 03:06:17 GMT	1mins, 5sec

View and Control Services on Each Host

westus-g1.westus-g1.d1.internal.cloudapp.net No alerts

[Back](#)

Summary [Configs](#)

Host Actions

Components + Add

✓ DataNode / HDFS

Started

✓ Ganglia Monitor / Ganglia

Started

✓ NodeManager / YARN

Started

Clients / HDFS Client , MapReduce2 Client , YARN Client , ZooKeeper Client

Installed

Summary

Hostname:

westus-g1.westus-g1.d1.internal.cloudapp.net

IP Address:

172.24.60.5

OS:

centos6 (x86_64)

Cores (CPU):

4 (4)

Disk:

53.6GB/873.04GB (6.14% used)

Memory:


55.15GB

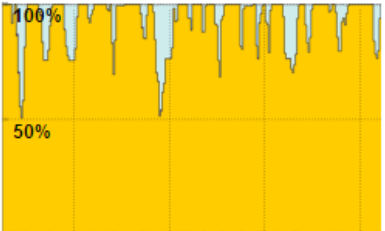
Load Avg:

4.01

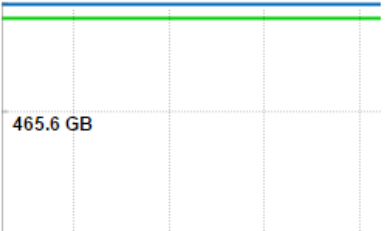
Heartbeat:

a moment ago

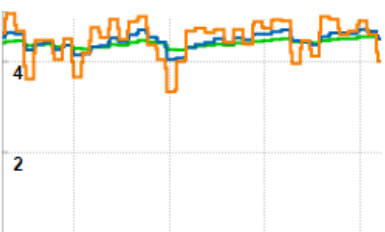
Host Metrics 



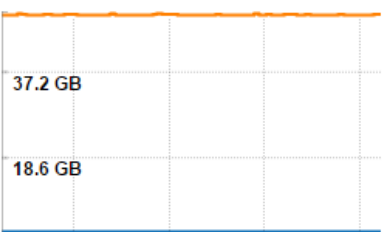
CPU Usage



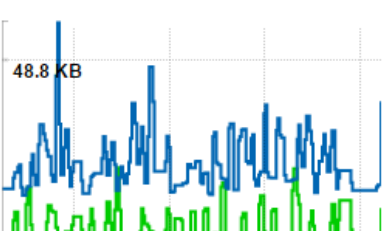
Disk Usage



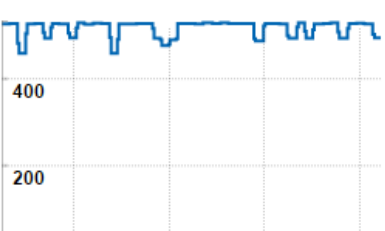
Load



Memory Usage

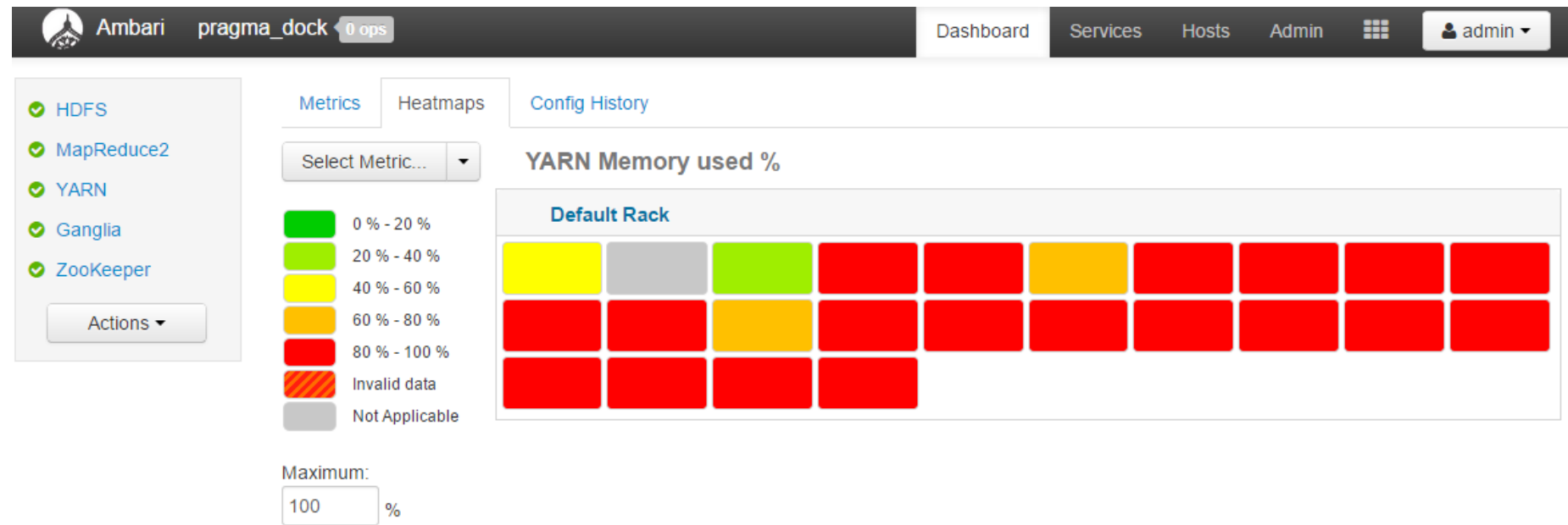


Network Usage



Processes

Lookup Service Usage via Heatmaps



Questions?

Acknowledgements



Thank you!