



BDU Cluster User Training

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HPC Engineer



Agenda

1

Overview of HPC Setup

2

Introduction to Job scheduler (SLURM) : Job Submitting & Monitoring

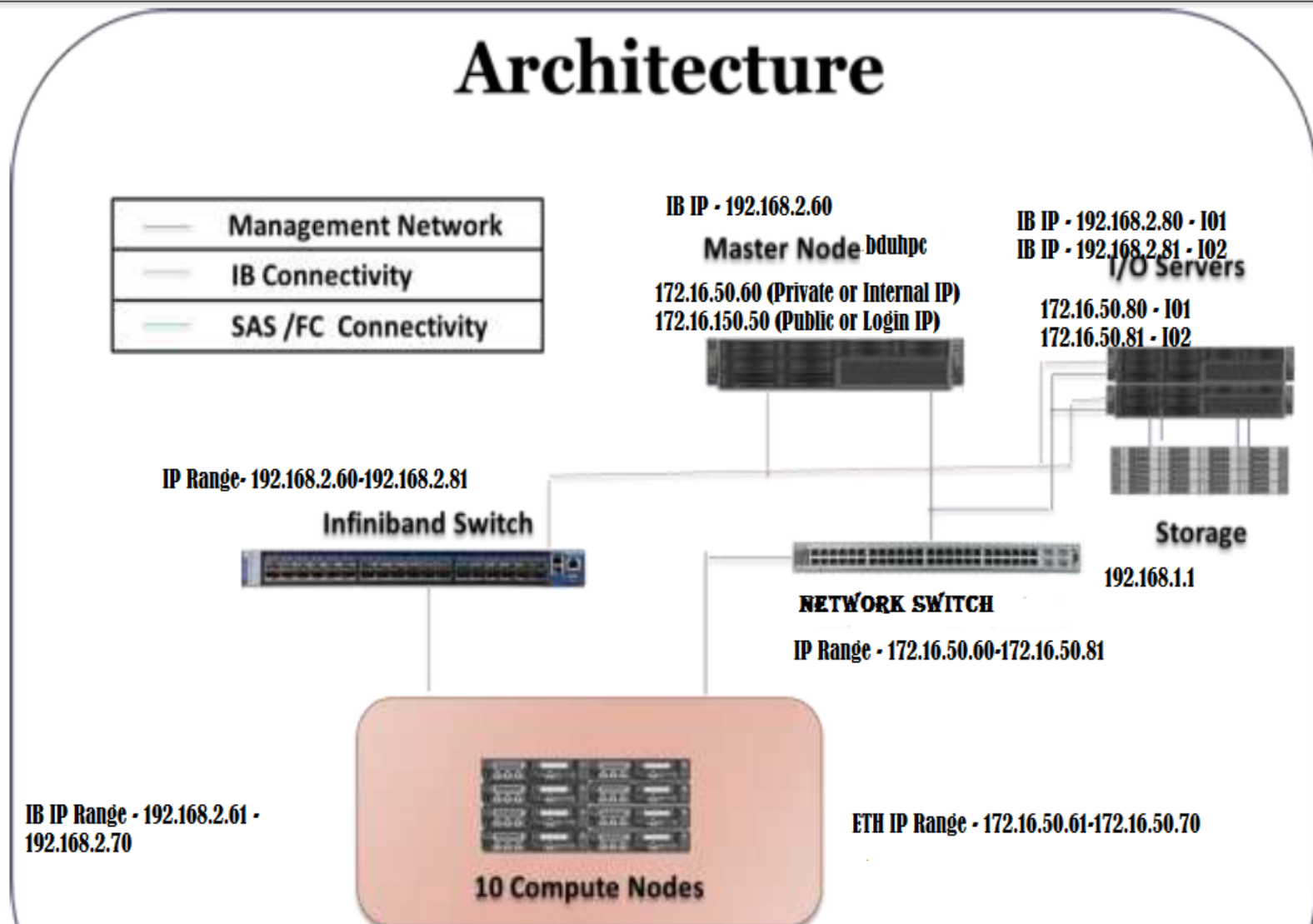
3

MPI and Libraries Paths

4

Wipro Job submission Portal & Ganglia

Cluster Architecture



Components

- **Master Node : 1 no**
- **Compute Nodes : 10 no's**
- **I/O Nodes : 2 no's**
- **Gigabit Switch : 1 no**
- **Infiniband Switch : 1 no**
- **Storage : 1 no**

HPC Setup Info

Details	Master node	Compute nodes	IO nodes
CPU Type	Intel Xeon E5-2670v2 @2.5 GHz	Intel Xeon E5-2670v2 @2.5 GHz	Intel Xeon E5-2660v2 @2.2 GHz
GPU Type	Not Applicable	Not Applicable	Not Applicable
No of CPUs/ Cores	2/10	2/10	2/10
No of GPU / node	Not Applicable	Not Applicable	Not Applicable
RAM	128GB DDR3	64GB DDR3	64GB DDR3
HDD	4 x300GB SAS hard disk	2 x 500GB SATA hard disk	2 x 500GB SATA hard disk
OS	CENTOS 6.5 64 bit	CENTOS 6.5 64 bit	CENTOS 6.5 64 bit
Partitions	Master Node	Compute Node	
/	630 GB	260 GB	
Swap	104 GB	104 GB	
/boot	500 MB	500 MB	
/boot/efi	500 MB	500 MB	
/storage	6.1 TB (Mounted from IONode1)	6.1 TB (Mounted from IONode1)	
/home	10 TB (Mounted from IONode1)	10 TB (Mounted from IONode1)	
/opt	2 TB (Mounted from IONode1)	2 TB (Mounted from IONode1)	
/var	100 GB	100 GB	

How to login to cluster

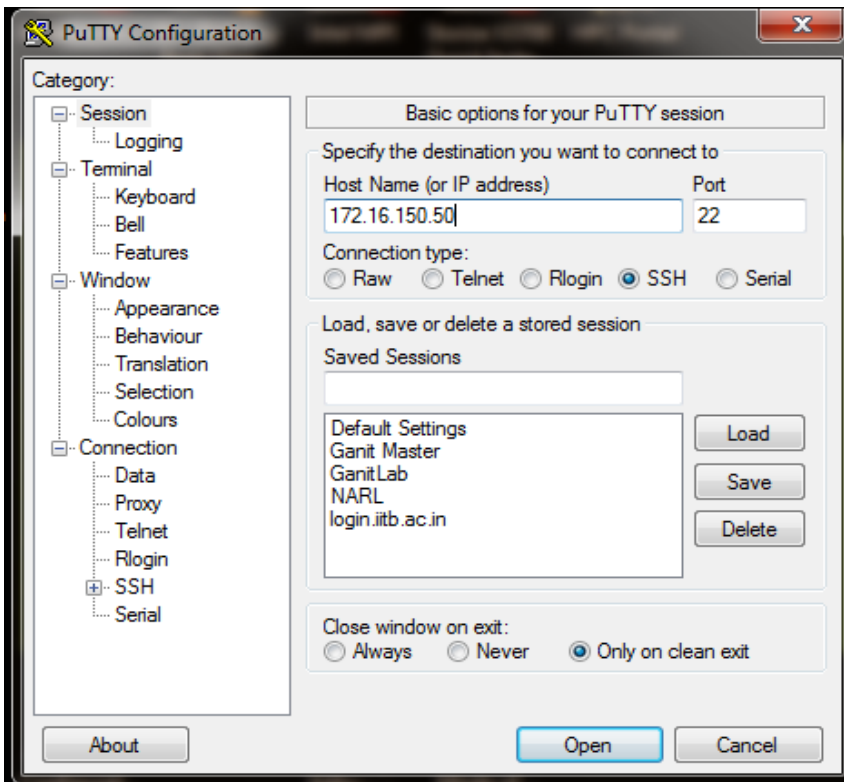
- Users can be able to login from anywhere at BDU LAN, where SSH is enabled. So users can simply do ssh from their systems

ssh 172.16.150.50

username : xxxxxxxxxxxxxxxx

password : xxxxxxxxxxxxxxxx

Login from BDU Network



From any linux machine users can login directly

ssh username@172.16.150.50

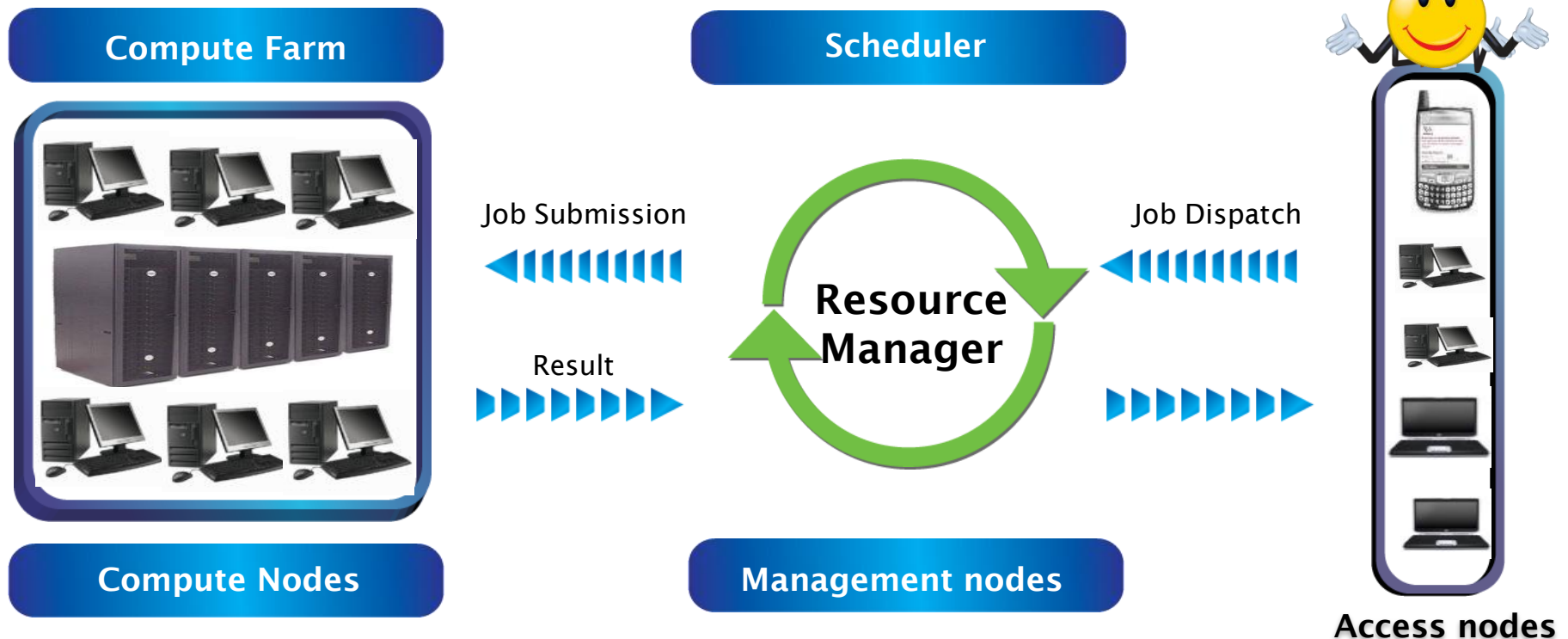
password : xxxxxxxxxxxxxxxx

IP addresses and Hostnames

- #####Network IP Lists#####
- 172.16.50.60 bduhpc bduhpc.bdu.ac.in
- 172.16.50.61 node1 node1.bdu.ac.in
- 172.16.50.62 node2 node2.bdu.ac.in
- 172.16.50.63 node3 node3.bdu.ac.in
- 172.16.50.64 node4 node4.bdu.ac.in
- 172.16.50.65 node5 node5.bdu.ac.in
- 172.16.50.66 node6 node6.bdu.ac.in
- 172.16.50.67 node7 node7.bdu.ac.in
- 172.16.50.68 node8 node8.bdu.ac.in
- 172.16.50.69 node9 node9.bdu.ac.in
- 172.16.50.70 node10 node10.bdu.ac.in
- 172.16.50.80 ionode1 ionode1.bdu.ac.in
- 172.16.50.81 ionode2 ionode2.bdu.ac.in
-
- ##### IB Network #####
- 192.168.2.60 bduhpc-ib
- 192.168.2.61 node1-ib
- 192.168.2.62 node2-ib
- 192.168.2.63 node3-ib
- 192.168.2.64 node4-ib
- 192.168.2.65 node5-ib
- 192.168.2.66 node6-ib
- 192.168.2.67 node7-ib
- 192.168.2.68 node8-ib
- 192.168.2.69 node9-ib
- 192.168.2.70 node10-ib
- 192.168.2.80 ionode1-ib
- 192.168.2.81 ionode2-ib

Slurm Architecture

- Slurm is a powerful workload management platform for demanding, distributed HPC environments. It provides a comprehensive set of intelligent, policy-driven scheduling features that enable you to utilise all of your compute infrastructure resources and ensure optimal application performance.



Slurm Architecture

- A SLURM cluster consists of one head/master node and 10 compute nodes.
- The master node runs the slurmd(daemon) & slurmdbd(database daemon) daemon and the compute nodes run the slurmd daemon.
- Client commands for submitting and managing jobs can be installed on any host .

SLURM Commands

Frequently Used Commands

Usage

- **sinfo** : Report system or Node status
- **sbatch** : Submit a batch job
- **squeue** : Report the status of jobs
- **scancel** : To cancel a job

- Detail job info – `scontrol show jobs <job id>`
- Detail Node Info – `scontrol show node`

How to Submit and monitor Node status

```
test@bduhpc~
```

```
[test@bduhpc ~]$ sinfo
```

```
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
CPU*      up    infinite    10   idle* node[1-10]
```

```
[test@bduhpc ~]$ sbatch namd.sh
```

```
Submitted batch job 177
```

```
[test@bduhpc ~]$ squeue
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST (REASON)
177	CPU	namd-job	test	PD	0:00	2	(Resources)

```
[test@bduhpc ~]$
```

- Submitting Namd job by user “test”

Software and Application installed

MPI Path:

- Installed Path = /opt/openmpi-1.8.8
- Installed Path = /opt/intel/impi

Applications and Libraries Path:

- SLURM-14.11.17 : /opt/slurm
- NAMD-2.9 : /home/test/namd
- Mvapich2.2 : /opt/mvapich2
- FFTW : /usr/bin/fftw-3.2.1

NAMD Submission script

```
root@bduhpc:/home/test
[root@bduhpc test]# cat namd.sh
#!/bin/sh

#SBATCH --job-name=namd-job
#SBATCH --output=namd-%J.out
#SBATCH --error=namd-%J.out
#SBATCH --workdir=/home/test
#SBATCH --ntasks-per-node=8
#SBATCH --nodes=2
#SBATCH --partition=CPU
cd /home/test/namd/apoal
MACHINE_FILE=/home/test/machinefile
scontrol show hostname $SLURM_JOB_NODELIST &> $MACHINE_FILE
/opt/intel/impi/5.0.3.048/intel64/bin/mpirun -np 16 -machinefile $MACHINE_FILE /home/test/namd/NAMD_2.9_Linux-x86_64/namd2 apoal.namd
[root@bduhpc test]#
```

WHPC Job Submission Portal

The screenshot shows a Mozilla Firefox browser window with the title "Wipro's Job Submission Portal - Mozilla Firefox". The address bar displays "172.16.150.50:8080/whpc-portal/pages/Login.faces". The page content includes the Wipro logo on the left and a "Welcome to Wipro's HPC Portal" message in the center. Below the welcome message is a "User Login" form with fields for "User Name:" (containing "root") and "Password:" (containing "*****"). There are "Login" and "Reset" buttons, and links for "Forgot password" and "New User". Below the login form is a "Declaration" box containing copyright information for 2013. The browser's taskbar at the bottom shows several open windows, including "TeamViewer" and multiple instances of "root@bduh...". A decorative graphic with colorful wavy lines is at the bottom of the page, with the text "2013-15 Copyright Wipro Ltd. | www.wipro.com | Built on Java Technologies" overlaid.

Applications Places System 86 °F Sat Aug 29, 2:41 PM root

Wipro's Job Submission Portal - Mozilla Firefox

File Edit View History Bookmarks Tools Help

Welcome to CentOS Wipro's Job Submission Portal

172.16.150.50:8080/whpc-portal/pages/Login.faces Google

 WIPRO Applying Thought

Welcome to Wipro's HPC Portal

User Login

User Name: *

Password: *

[Forgot password](#)
[New User](#)

Declaration

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[test@bduh...] [root@bduh...] [TeamViewer] [root@bduh...] [root@bduh...] [root@iono...] [Ganglia:: b... root@bduh... root@bduh... Wipro's Job ...

Login Page

User Addition Page

The screenshot shows a web browser window titled "Wipro's Job Submission Portal - Mozilla Firefox". The address bar shows the URL "172.16.150.50:8080/whpc-portal/pages/secured/admin/Users.xhtml". The page content includes a sidebar with navigation links like "Manage Apps" and "Other". The main area shows a "Welcome to Wipro's HPC Portal" message and a table of users. An "Add User" modal form is open, allowing the addition of a new user.

Table: Overview Users

Index	User Name	E-mail Address	Contact Number	Name	Department	User Role	Last Login	Last Logout	Last Session Id
1	root	root@localhost		root root			24		373C6F2D09E9C017BA2F965ACFD88D87

Add User Modal Form:

- User Role*: User
- Department*: General
- User name*: test
- First name*: test
- Last name*: test
- E-mail*: test.com
- Mobile Number:
- Date Of Birth*:

Buttons: Add User, Reset

Users Detail Page

Applications Places System 82 °F Wed Sep 2, 12:44 AM root

Wipro's Job Submission Portal - Mozilla Firefox

File Edit View History Bookmarks Tools Help

Wipro's Job Submission Portal

172.16.150.50:8080/whpc-portal/pages/secured/admin/Users.xhtml Google

Welcome to Wipro's HPC Portal Wipro

Home Monitoring History Statistics Ganglia Documentation Hello, root!

Manage Apps

- Cluster
- Domain
- Compilers
- Applications
- Application Execution

Other

- User
- Notices
- Department

Overview Users ▶ User Details

Index	User Name	E-mail Address	Contact Number	Name	Department	User Role	Last Login	Last Logout	Last Session Id
1	root	root@localhost		root root	General	Administrator	2015-09-02 00:43:40	2015-09-02 00:39:37	6110C31226274D76FF73A5350E390B79
2	test	test@test.com		test test	General	User	2015-09-02 00:39:45	2015-09-02 00:43:31	FB5FD65B2C85EA794B3DEAFCFE1D0D2D

Add

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root@bduhpc:~ [TeamViewer] Wipro's Job Sub... test@bduhpc:~ root@node1:~ root@bduhpc:~ Sponsored ses... TeamViewer - ...

Statistics Module Users Wise



Welcome to Wipro's HPC
Portal

[Home](#) [Monitoring](#) [History](#) [Statistics](#) [Ganglia](#)

By Users ▼

All Clusters ▼

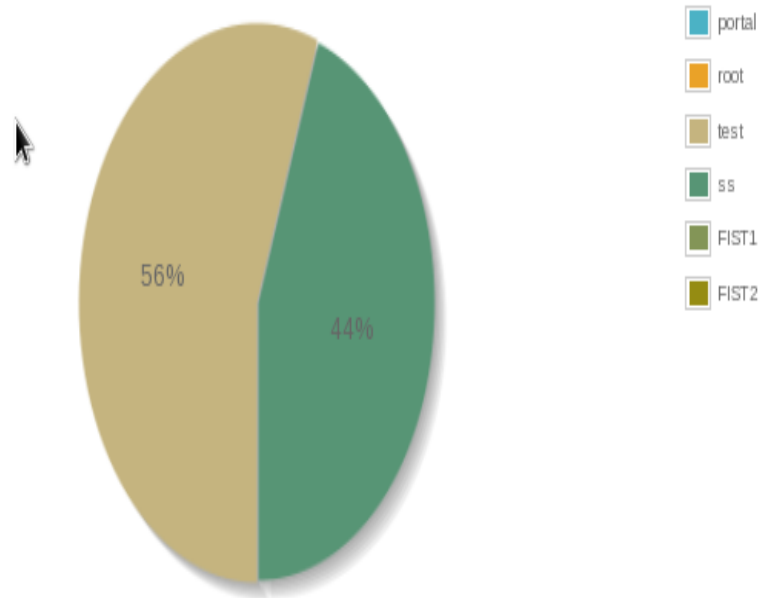
Select Users ▼

Fort Night ▼

Total No. Of Jobs By Users

Export Plot As Image

Export



Ganglia

A ganglia is the tool that provides the various information regarding the status of the Cluster. This information can be accessed through a web browser. The below IP address provide the access to this Monitoring tool.

This monitor gathers various metrics such as CPU load, free memory, disk usage, etc. These metrics are sent through the private cluster network and are used by the frontend n to generate the data in a graphical manner

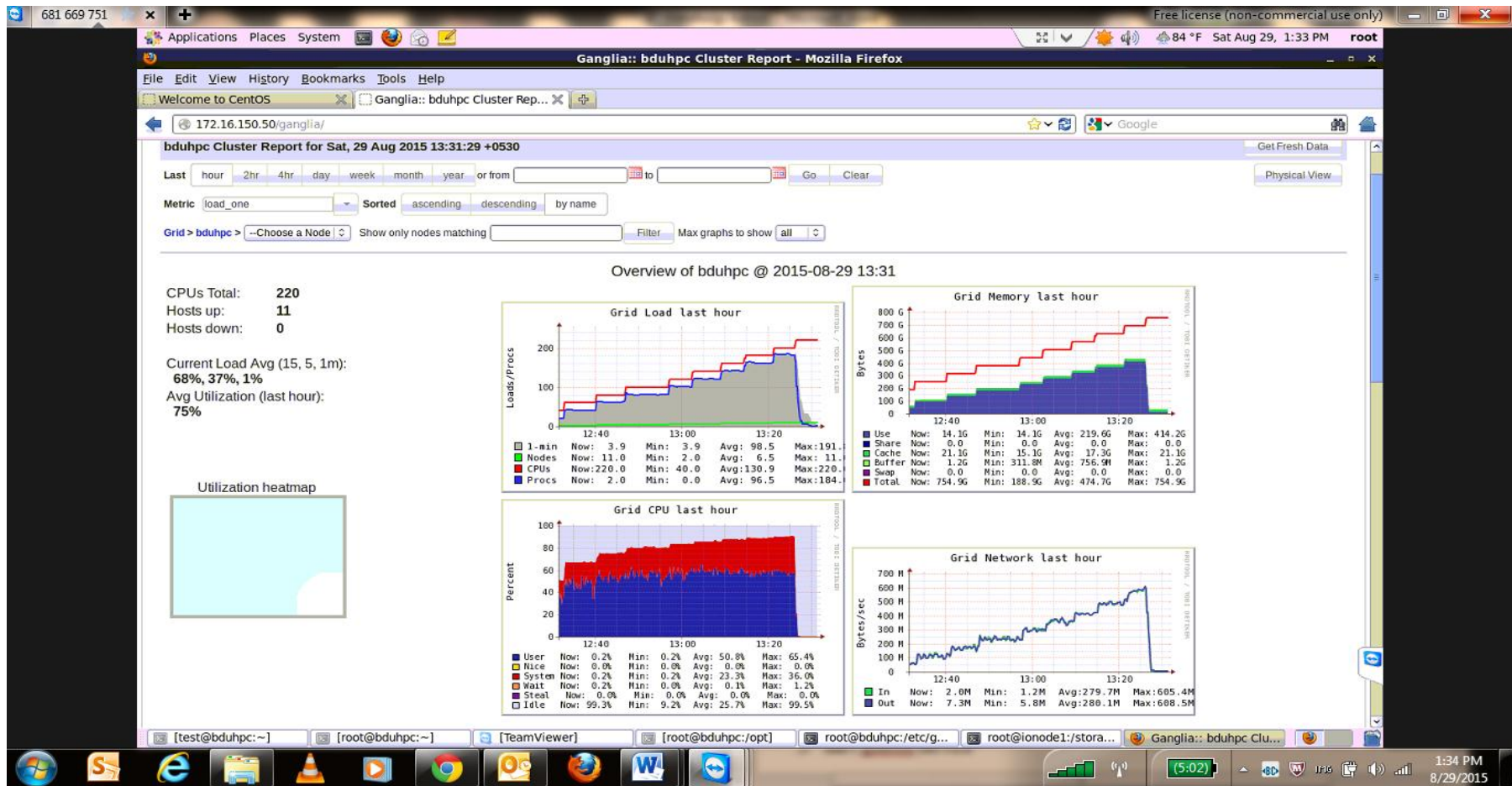
In addition to metric parameters, a heartbeat message from each n is collected by the Ganglia. When certain number of heartbeats from any n is missed, this web page will declare it "dead".

Link to access :<http://172.16.150.50/ganglia>

For individual hosts, you can see the details of following values:

Bytes_in	5) cpu_system	9) proc_run
Bytes_out	6) cpu_user	10) proc_total
cpu_idle	7) disk_free	11) swp_free
cpu_nice	8) packets_in	

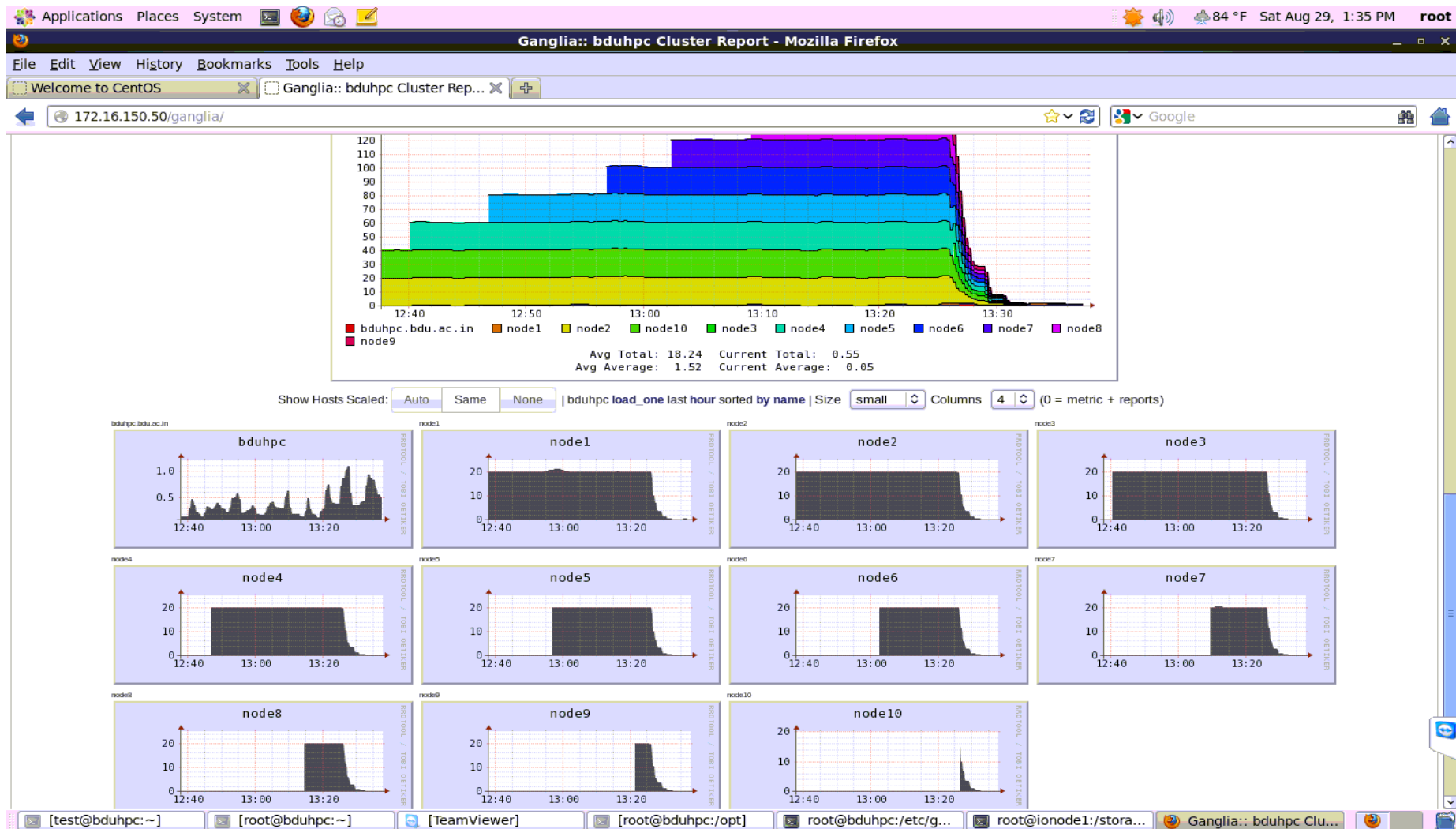
Grid Structure



Grid Structure :

- Total CPU/Cores
- Total Hosts Up
- Total Hosts Down

Graphical Statistics of Nodes



How to log a call with Wipro

- **Log a call with Wipro on below mail ID:**

upamanyu.ghosh@wipro.com

or

hpc-support@wipro.com

Questions..?





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,
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