Kohinoor Cluster User/Admin Manual

Intel Xeon 272 Cores HPC Cluster

At

Tata Institute of Fundamental Research [TIFR]

Hyderabad

By

Locuz Enterprise Solutions Ltd

6th floor, Office no 4, Orion towers,
Building #9, Mindspace, Cyberabad,
Madhapur, Hyderabad– 500081.

Contents

Chapter 1

About Document

1.1. Document History

Version	Release Date	Prepared by
1.0	11th Sept 2012	Locuz Enterprise Solution Ltd

1.2. Locuz Contact Details

Please refer page number for "Support Escalation Matrix"

1.3. Target Group

This document is designed for End-Users for reference of technical and usage details. In this document, it has been tried to provide a clear-cut theoretical picture and practical approach to use the cluster in a better way.

1.4. Typographic Conventions

Four typographic conventions are used to call attention to specific words and phrases. These conventions, and the circumstances they apply to, are as follows:

Arial 16 Bold Centered

Used to specify Chapter Headings

Trebuchet MS 12 Bold

Used to specify side-headings and sub-headings in a chapter with/without sub-heading number

<u>Trebuchet MS 12 Bold</u>
Trebuchet MS 12 Bold

Used to specify the heading that is again a sub-heading of a side-heading

`Courier New 12 Bold` or `Courier New 12`

Used to specify the system commands and output

Chapter 2

Introduction

2.1. About Clustering

A computer cluster is a group of linked computers, working together closely thus in many respects forming a single computer. The components of a cluster are commonly, but not always, connected to each other through fast local area networks. Clusters are usually deployed to improve performance and availability over that of a single computer, while typically being much more cost-effective than single computers of comparable speed or availability.

Cluster categorizations

a. Compute clusters:

Often clusters are used primarily for computational purposes, rather than handling IO-oriented operations such as web service or databases. For instance, a cluster might support computational simulations of weather or vehicle crashes. The primary distinction within computer clusters is how tightly-coupled the individual nodes are. For instance, a single computer job may require frequent communication among nodes - this implies that the cluster shares a dedicated network, is densely located, and probably has homogenous nodes. This cluster design is usually referred to as Beowulf Cluster. The other extreme is where a computer job uses one or few nodes, and needs little or no inter-node communication. This latter category is sometimes called "Grid" computing. Tightly-coupled compute clusters are designed for work that might traditionally have been called "supercomputing". Middleware such as MPI (Message Passing Interface) or PVM (Parallel Virtual Machine) permits compute clustering programs to be portable to a wide variety of clusters.

2.2. High-Performance Computing (HPC):

High-performance computing (HPC) uses supercomputers and computer clusters to solve advanced computation problems. Today, computer systems approaching the teraflops-region are counted as HPC-computers.

HPC integrates systems administration and parallel programming into a multidisciplinary field that combines digital electronics, computer architecture, system software, programming languages, algorithms and computational techniques. HPC technologies are the tools and systems used to implement and create high performance computing systems.

Recently, HPC systems have shifted from supercomputing to computing clusters and grids. Because of the need of networking in clusters and grids, High Performance Computing Technologies are being promoted by the use of a collapsed network backbone, because the collapsed backbone architecture is simple to troubleshoot and upgrades can be applied to a single router as opposed to multiple ones.

The term is most commonly associated with computing used for scientific research or computational science. A related term, high-performance technical computing (HPTC), generally refers to the engineering applications of cluster-based computing (such as computational fluid dynamics and the building and testing of virtual prototypes). Recently, HPC has come to be applied to business uses of cluster-based supercomputers, such as data warehouses, line-of-business (LOB) applications, and transaction processing.

High-performance computing (HPC) is a term that arose after the term "supercomputing." HPC is sometimes used as a synonym for supercomputing; but, in other contexts, "supercomputer" is used to refer to a more powerful subset of "high-performance computers," and the term "supercomputing" becomes a subset of "high-performance computing." The potential for confusion over the use of these terms is apparent.

Because most current applications are not designed for HPC technologies but are retrofitted, they are not designed or tested for scaling to more powerful processors or machines. Since networking clusters and grids use multiple processors and computers, these scaling problems can cripple critical systems in future supercomputing systems. Therefore, either the existing tools do not address the needs of the high performance computing community or the HPC community is unaware of these tools. A few examples of commercial HPC technologies are the simulation of car crashes for structural design, molecular interaction for new drug design and the airflow over automobiles or airplanes. In government and research institutions, scientists are simulating galaxy creation, fusion energy, and global warming, as well as working to create more accurate short- and long-term weather forecasts.

2.3. HPC Stack:

HPC Stack is a cluster components’ stack which explains about different components which uses in HPC cluster implementation and its dependencies on one another. Figure 2.1 shows a brief view about components and its dependency.

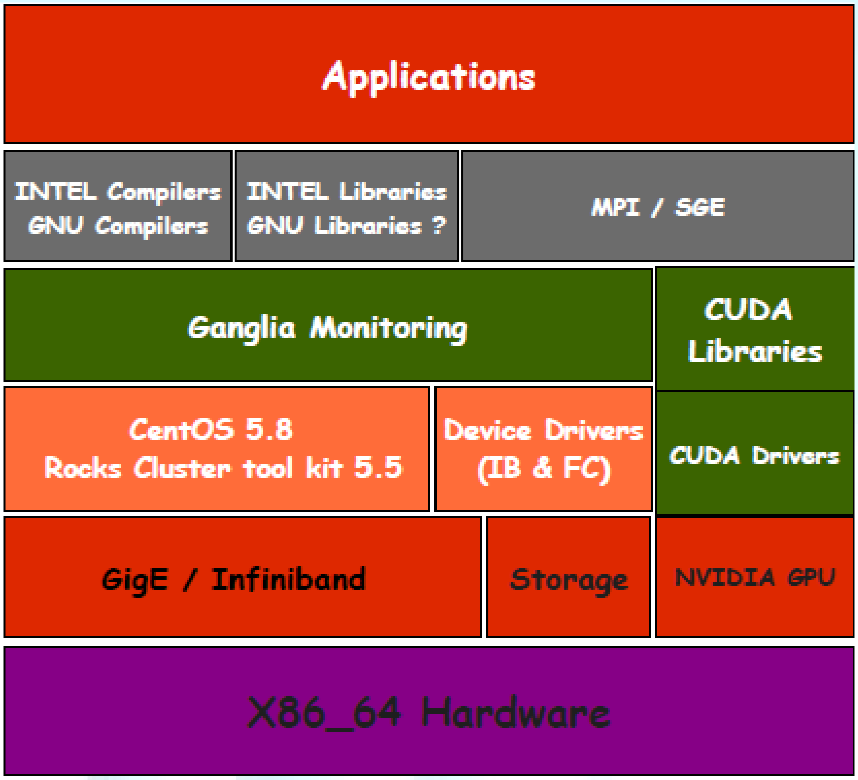


Figure 2.1: HPC Stack

a. *Hardware:*

Servers: 32-bit/64-bit servers, which generally have rich hardware resources like Multi-core processors, RAM, Storage, etc.

Storage: Storage may be internal, which is attached to Master node internally i.e. internal HDDs or external. Generally external storage can be configured for home directory and backup

Ethernet: Ethernet provides a conventional intercommunication among all nodes. This requires Ethernet NIC, Ethernet switch and its cables.

Infiniband: Infiniband gives much faster communication than conventional Ethernet communication. It improves the job execution speed and inter-node communication. To configure Infiniband, setup requires three things – Infiniband Cards, Infiniband switch and its cables.

HPC hardware is combination of at least one Master Node, many Compute Nodes, Storage, Network and Storage Switches, connectivity channels/cables, etc. Master node is a special server which plays an administrator role for whole cluster. It provides a centralized facility to create/delete users, create ACLs, and define roles for different compute nodes, installation of software and many administrative activities. It is mandatory for any HPC cluster that one node should be master node but according to requirement, it can be configuring more than one master node.

In Kohinoor implementation, the cluster has been configured with Single master nodes configuration.

b. *Operating System:*

Operating System plays a great foundational role in cluster configuration. OS manages all resources properly according to specifications and configuration. Apart from hardware management, it is mandatory to create and configure some special things like ssh password-free environment, centralized home directory management, synchronization of user information, facility to execute commands concurrently across the cluster nodes, etc.

On top of Kohinoor server hardware, Rocks cluster 5.5 mamba has been installed with CentOS 5.8 Operating system.

c. *Libraries:*

Library is a collection of resources used to develop software. These may include pre-written code and subroutines, classes, values or type specifications. Libraries contain code and data that provide services to independent programs. This allows the sharing and changing of code and data in a modular fashion. Some executables are both standalone programs and libraries, but most libraries are not executable. Executables and libraries make references known as links to each other through the process known as linking, which is typically done by a linker.

Here in HPC Stack, libraries mean development libraries both serial and parallel which are associated with compilers and other HPC programs to run jobs.

Originally, only static libraries existed. A static library, also known as an archive, consists of a set of routines which are copied into a target application by the compiler, linker, or binder, producing object files and a stand-alone executable file. This process, and the stand-alone executable file, is known as a static build of the target application. Actual addresses for jumps and other routine calls are stored in a relative or symbolic form which cannot be resolved until all code and libraries are assigned final static addresses.

Dynamic linking involves loading the subroutines of a library into an application program at load time or run-time, rather than linking them in at compile time. Only a minimum amount of work is done at compile time by the linker; it only records what library routines the program needs and the index names or numbers of the routines in the library. The majority of the work of linking is done at the time the application is loaded (load time) or during execution (runtime).

In addition to identifying static and dynamic loading, computer scientists also often classify libraries according to how they are shared among programs. Dynamic libraries almost always offer some form of sharing, allowing the same library to be used by multiple programs at the same time. Static libraries, by definition, cannot be shared.

With CentOS 5.8 on Kohinoor, glibc is installed for OS and developmental activities.

The GNU C Library, commonly known as glibc, is the C standard library released by the GNU Project. Originally written by the Free Software Foundation (FSF) for the GNU operating system, the library's development has been overseen by a committee since 2001, with Ulrich Drepper from Red Hat as the lead contributor and maintainer.

d. *Compilers:*

A compiler is a computer program (or set of programs) that transforms source code written in a programming language (the source language) into another computer language (the target language, often having a binary form known as object code). The most common reason for wanting to transform source code is to create an executable program.

The GNU Compiler Collection (GCC) is a compiler system produced by the GNU Project supporting various programming languages. GCC is a key component of the GNU tool chain. As well as being the official compiler of the unfinished GNU operating system, GCC has been adopted as the standard compiler by most other modern Unix-like computer operating systems, including Linux, the BSD family and Mac OS X.

Originally named the GNU C Compiler, because it only handled the C programming language, GCC 1.0 was released in 1987, and the compiler was extended to compile C++ in December of that year. Front ends were later developed for FORTRAN, Pascal, Objective-C, Java, and Ada, among others.

e. *Scheduler:*

A job scheduler is a software application that is in charge of unattended background executions, commonly known for historical reasons as batch processing. Synonyms are batch system, Distributed Resource Management System (DRMS), and Distributed Resource Manager (DRM). Today's job schedulers typically provide a graphical user interface and a single point of control for definition and monitoring of background executions in a distributed network of computers. Increasingly job schedulers are required to orchestrate the integration of real-time business activities with traditional background IT processing, across different operating system platforms and business application environments.

Basic features expected of job scheduler software are: Interfaces which help to define workflows and/or job dependencies, automatic submission of executions, interfaces to monitor the executions and priorities and/or queues to control the execution order of unrelated jobs.

An important niche for job schedulers is managing the job queue for a cluster of computers. Typically, the scheduler will schedule jobs from the queue as sufficient resources (cluster nodes) become idle. Some widely used cluster batch systems are Sun Grid Engine, Portable Batch System, Load Leveler, Condor, OAR and Simple Linux Utility for Resource Management.

For Kohinoor resources management, Sun Grid Engine v6.2 is a open-source HPC job scheduler. Now it is Oracle Grid Engine, previously known as Sun Grid Engine (SGE) is an open source batch-queuing system, developed and supported by Sun Microsystems. Sun once also sold a commercial product based on SGE, known as N1 Grid Engine (N1GE). SGE is typically used on a computer farm or high-performance computing (HPC) cluster and is responsible for accepting, scheduling, dispatching, and managing the remote and distributed execution of large numbers of standalone, parallel or interactive user jobs. It also manages and schedules the allocation of distributed resources such as processors, memory, disk space, and software licenses.

f. *Monitoring Tools:*

A system monitor or monitoring tool is hardware or software-based system used to monitor resources and performance in a computer system.

Ganglia is a scalable distributed system monitor tool for high-performance computing systems such as clusters and grids. It allows the user to remotely view live or historical statistics (such as CPU load averages or network utilization) for all machines that are being monitored.

g. *MPI:*

Message Passing Interface (MPI) is an API specification that allows processes to communicate with one another by sending and receiving messages. Besides many other applications, it is a de facto standard for parallel programs running on computer clusters and supercomputers, where the cost of accessing non-local memory is high. MPI was created since 1992 by William Gropp, Ewing Lusk and others, a first standard appeared in 1994.

MPI is a language-independent communications protocol used to program parallel computers. Both point-to-point and collective communication are supported. MPI "is a message-passing application programmer interface, together with protocol and semantic specifications for how its features must behave in any implementation." MPI's goals are high performance, scalability, and portability. MPI remains the dominant model used in high-performance computing today.

At present, the standard has several popular versions: version 1.3 (shortly called MPI–1), which emphasizes message passing and has a static runtime environment, and MPI–2.2 (MPI–2), which includes new features such as parallel I/O, dynamic process management and remote memory operations.[5] MPI–2's LIS specifies over 500 functions and provides language bindings for ANSI C, ANSI Fortran (Fortran90), and ANSI C++. Object interoperability was also added to allow for easier mixed-language message passing programming. A side–effect of MPI–2 standardization (completed in 1996) was clarification of the MPI–1 standard, creating the MPI–1.2.

Note that MPI–2 is mostly a superset of MPI–1, although some functions have been deprecated. MPI–1.3 programs still work under MPI implementations compliant with the MPI–2 standard.

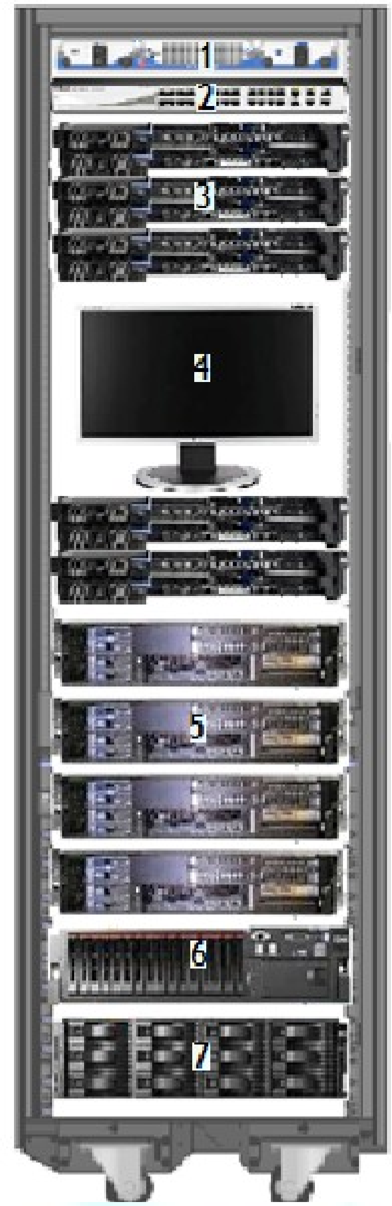
Open MPI is an Message Passing Interface (MPI) library project combining technologies and resources from several other projects (FT-MPI, LA-MPI, LAM/MPI, and PACX-MPI). It is used by many TOP500 supercomputers including Roadrunner, which was the world's fastest supercomputer from June 2008 to November 2009, and K computer, the fastest supercomputer since June 2011.

h. *Applications:*

Application program can be any program which can either run on individually on different nodes or on across the node in a parallelized manner. HPC applications are programs which may be designed by end-user or purchased from third party software vendors. Applications may be serial or parallel but this is all depends on the end-user and his requirement which decides.

Chapter 3

KOHINOOR Implementation



1. IB Switch
2. Ethernet Switch
3. Compute nodes
4. Monitor
5. GPU nodes
6. Master Node
7. Storage

Figure 3.1: KOHINOOR Rack Setup View

3.1. Servers Hardware Details

In KOHINOOR cluster, there is a single master node, 12 compute nodes and 4 GPU nodes. The following are the hardware details of Servers:

Master Node:

Hardware Details – IBM X3650 M4	
Processor	2 x Intel Xeon 8-core 2.4 GHz
RAM	64 GB DDR3
HDD	11 x 900 GB – 7200 RPM
Ethernet	4 ports
Serial Management	1 port
Net Management	1 port
Infiniband	1 port
FC	2 ports
Optical Drive	DVD Drive
OS Details	
OS	CentOS 5.8
Kernel	2.6.18-308.4.1.el5
Partition Details	
/	591 GB
Swap	32 GB
/export	190 GB
/export/home	5.6TB
/scratch	12TB
/scratch2	13TB

Compute Nodes: 12 Compute & 4 GPU nodes.

Hardware Details - IBM iDataplex DX 360 M4	
Processor	2 x Intel Xeon 8-core 2.4 GHz
RAM	32 GB DDR3
HDD	1 x 500 GB – 7200 RPM
Ethernet	2 ports
Net Management	1 port
InfiniBand	1 port

OS Details	
OS	CentOS 5.8
Kernel	2.6.18-308.4.1.el5
Partition Details	
/	419GB
Swap	32 GB
/boot	1GB
/export/data	190GB (nfs from master)
/scratch	12TB (nfs from master)
/scratch2	13TB (nfs from master)

3.2. Switches and Connectivity:

In Kohinoor implementation, two types of switches has been used – Ethernet, Infiniband switches.

Ethernet Switch:

In Kohinoor implementation, 24 Port Gigabit Dlink Switch has been used to configure the private network and in figure 3.2, Ethernet connectivity has been explained:

Dlink DGS-1210-24	
Type	Gigabit Switch
Speed	10/100/1000 Mbps
No.of Ports	24
Connectivity	Nodes are connected using CAT 6

Infiniband Switch:

In Kohinoor, one Infiniband switch with 36 ports for HPC Application/MPI communication. All the nodes including master have been IBSwitch.

The complete connectivity diagram among all hardware components has been explained by a schematic diagram in figure 3.3

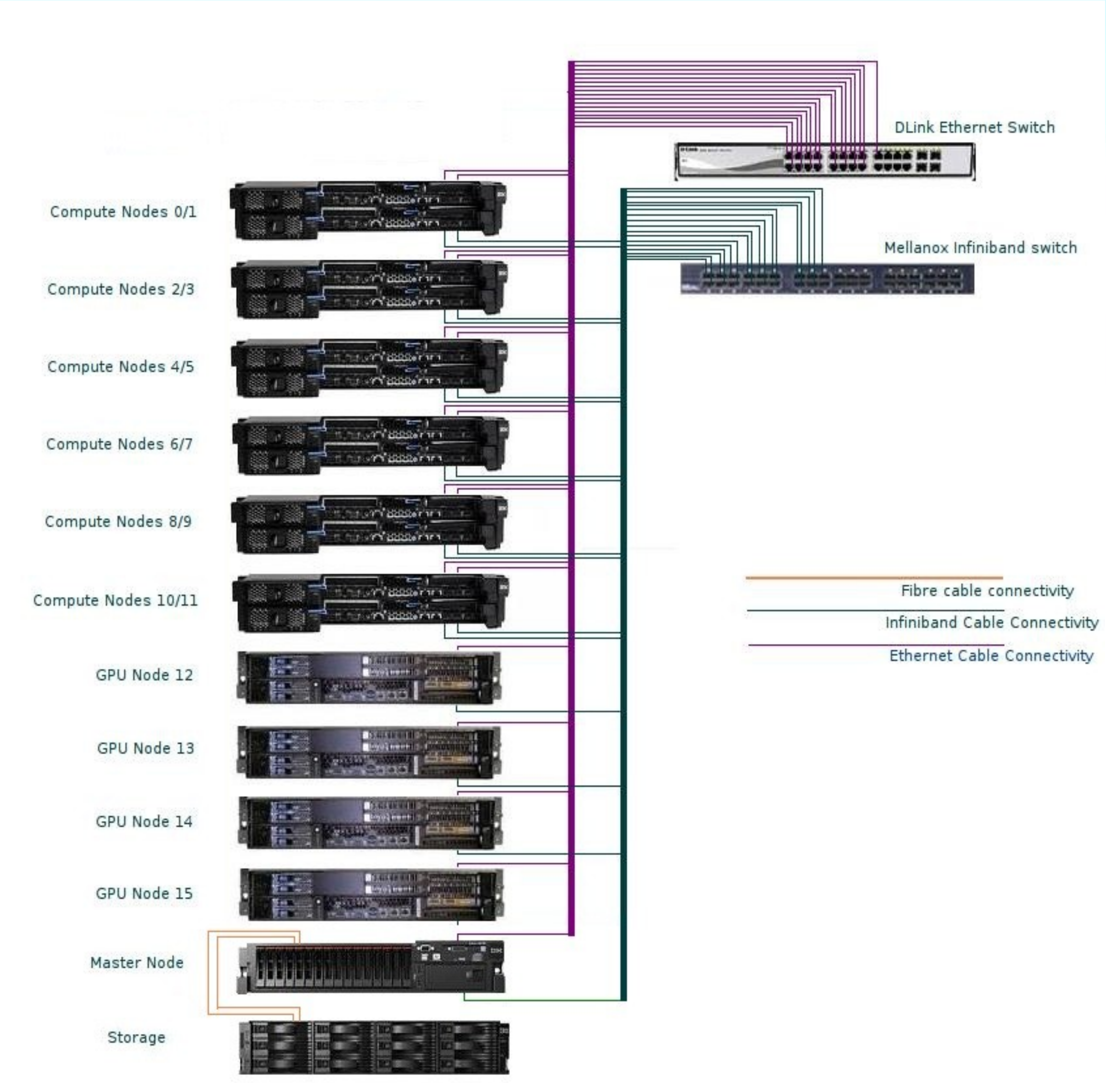


Figure 3.3: Kohinoor Schematic Diagram

The connectivity as explained above, the IP configuration details are:

SNo	Host Name	Gigabit Eth IP	IB IP	Mgmt IP	TIFR LAN IP
1	kohinoor	192.168.0.100	192.168.2.100	192.168.0.200	172.16.10.20
2.	node1	192.168.0.1	192.168.2.1	192.168.0.101	
3	node2	192.168.0.2	192.168.2.2	192.168.0.102	
4	node3	192.168.0.3	192.168.2.3	192.168.0.103	
5	node4	192.168.0.4	192.168.2.4	192.168.0.104	
6	node5	192.168.0.5	192.168.2.5	192.168.0.105	

7	node6	192.168.0.6	192.168.2.6	192.168.0.106	
8	node7	192.168.0.7	192.168.2.7	192.168.0.107	
9	node8	192.168.0.8	192.168.2.8	192.168.0.108	
10	node9	192.168.0.9	192.168.2.9	192.168.0.109	
11	node10	192.168.0.10	192.168.2.10	192.168.0.110	
12	node11	192.168.0.11	192.168.2.11	192.168.0.111	
13	node12	192.168.0.12	192.168.2.12	192.168.0.112	
14	gpunode1	192.168.0.13	192.168.2.13	192.168.0.113	
15	gpunode2	192.168.0.14	192.168.2.14	192.168.0.114	
16	gpunode3	192.168.0.15	192.168.2.15	192.168.0.115	
17	gpunode4	192.168.0.16	192.168.2.16	192.168.0.116	
18	storage	192.168.0.50			

3.3. Storage:

IBM System Storage DS3512 Express is a Single Controller Storage has been configured. IBM system storage client software has been installed in the master. 192.168.0.50 is the storage IP assigned. SMclient is the command to invoke the software at the master node.

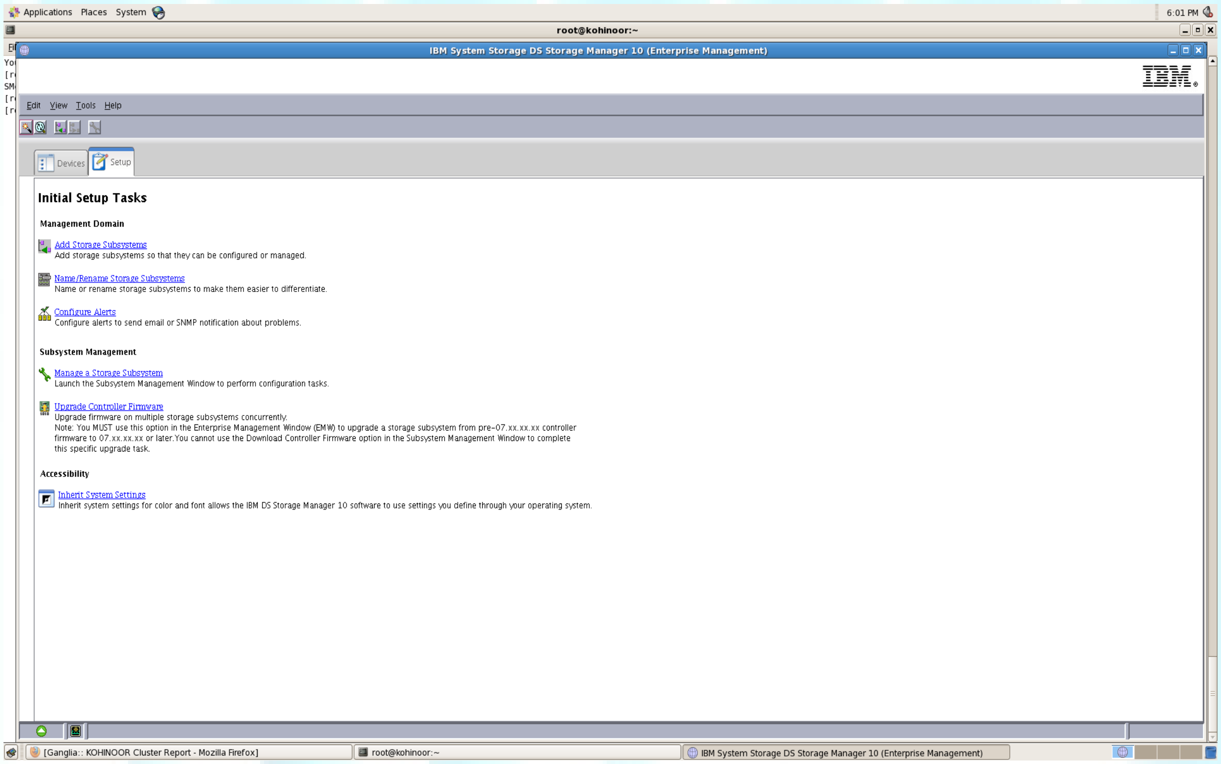
SMclient is the command to invoke the Storage Enterprise management console.

Enter the password which is same as root password to login in. From there we can access the Array management console by clicking on Manage Storage array option in Enterprise console

IBM System Storage DS3512 is a single Controller with 8 GB 4 ports Daughter Card and 2 SPF are attached. It has 753MB of Data cache & 7639MB of Cache backup device and 12 number of 3TB each NL SAS Drive.

Created a one logical array with RAID-5 associated 10 numbers of NL SAS drives, Total Storage capacity is 24.556TB associated 9 numbers of Data Disk and 1 Parity Disk in a RAID group.

Two luns has been created, its capacity 12TB and 12.555TB each and assigned to Master Server. The storage is connected to the master server through two fc cables.


Applications Places System
6:01 PM
root@kohinoor:~
IBM System Storage DS Storage Manager 10 (Enterprise Management)
IBM.
Edit View Tools Help
Devices
Setup
[Ganglia:: KOHINOOR Cluster Report - Mozilla Firefox]
root@kohinoor:~
IBM System Storage DS Storage Manager 10 (Enterprise Management)

Initial Setup Tasks

Management Domain

Add Storage Subsystems
Add storage subsystems so that they can be configured or managed.

Name/Rename Storage Subsystems
Name or rename storage subsystems to make them easier to differentiate.

Configure Alerts
Configure alerts to send email or SNMP notification about problems.

Subsystem Management

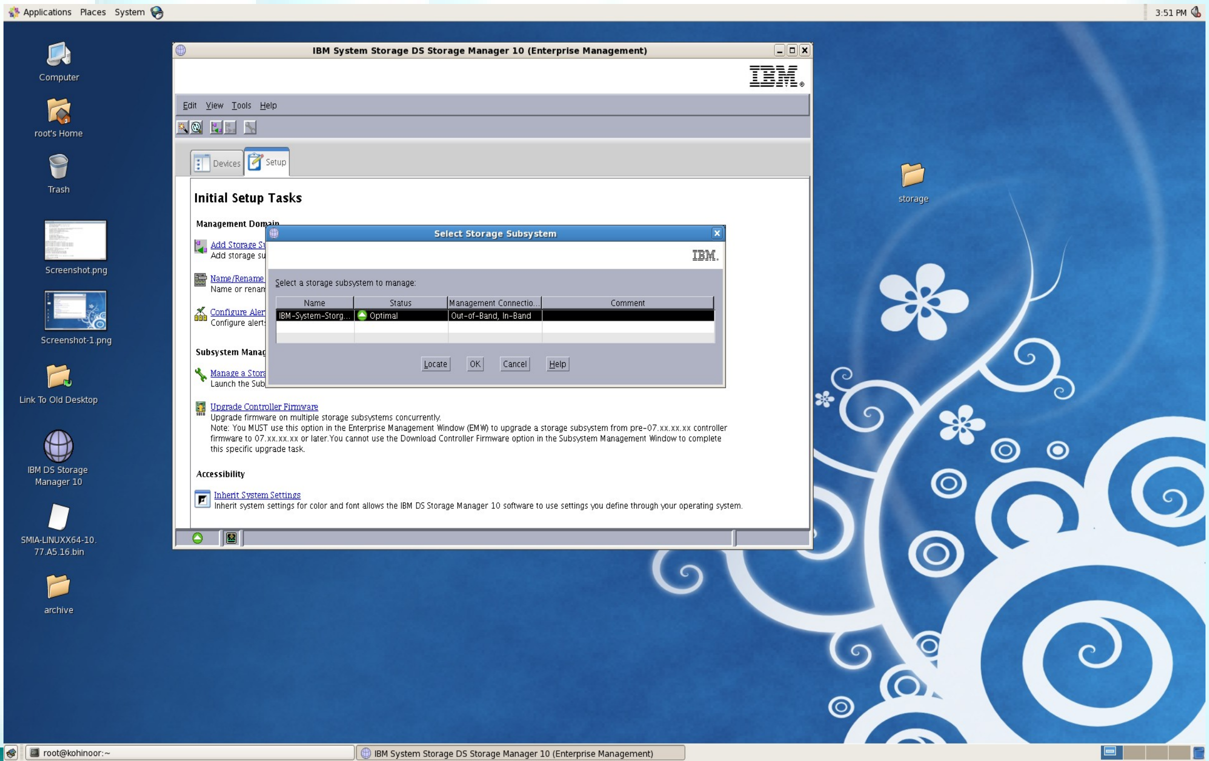
Manage a Storage Subsystem
Launch the Subsystem Management Window to perform configuration tasks.

Upgrade Controller Firmware
Upgrade firmware on multiple storage subsystems concurrently.
Note: You MUST use this option in the Enterprise Management Window (EMW) to upgrade a storage subsystem from pre-07.xx.xx.xx controller firmware to 07.xx.xx.xx or later.You cannot use the Download Controller Firmware option in the Subsystem Management Window to complete this specific upgrade task.

Accessibility

Inherit System Settings
Inherit system settings for color and font allows the IBM DS Storage Manager 10 software to use settings you define through your operating system.

Fig: Enterprise Console Management


Applications Places System
3:51 PM
Computer
root's Home
Trash
Screenshot.png
Screenshot-1.png
Link To Old Desktop
IBM DS Storage Manager 10
SMIA-LINUXX64-10.77.A5.16.bin
archive
storage
IBM System Storage DS Storage Manager 10 (Enterprise Management)
IBM.
Edit View Tools Help
Devices
Setup
Select Storage Subsystem
IBM.
Locate
OK
Cancel
Help
root@kohinoor:~
IBM System Storage DS Storage Manager 10 (Enterprise Management)

Initial Setup Tasks

Management Domain

Add Storage Su
Add storage su

Name/Rename
Name or renan

Configure Aler
Configure alert

Select a storage subsystem to manage:

Name	Status	Management Connectio...	Comment
IBM-System-Storg...	Optimal	Out-of-Band, In-Band	

Subsystem Manag

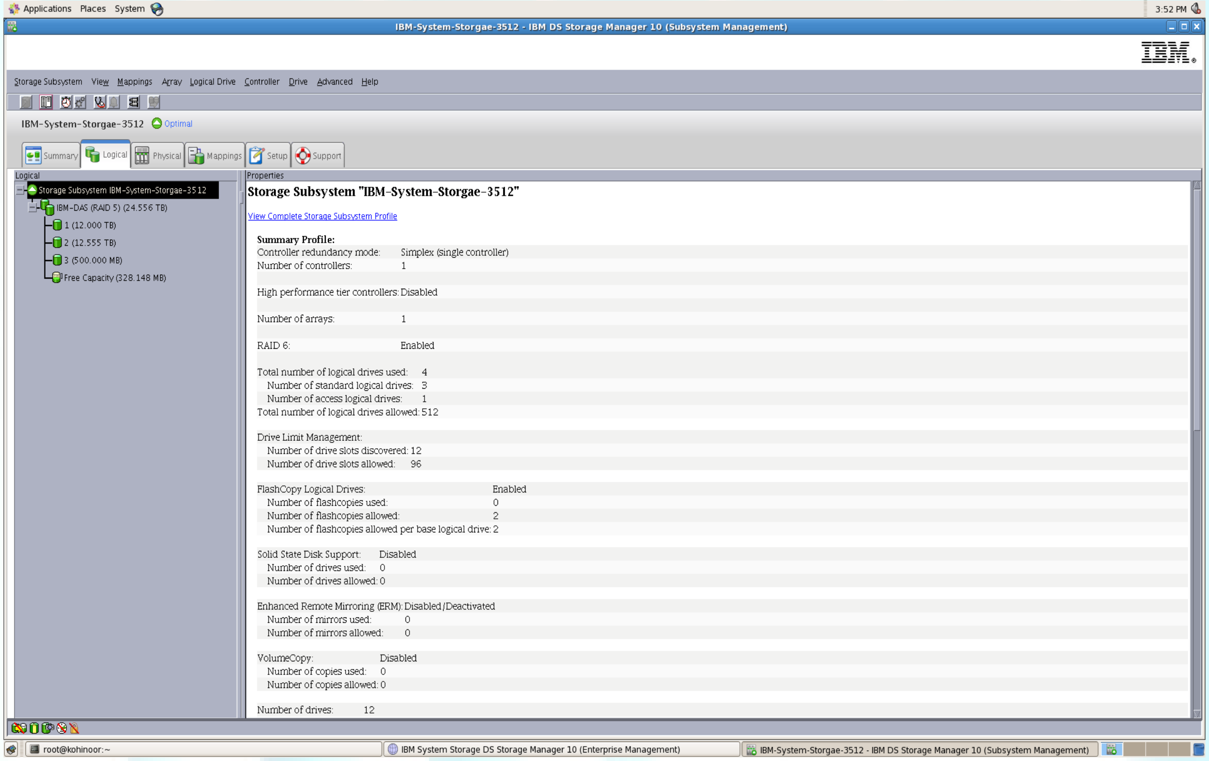
Manage a Stora
Launch the Sub

Upgrade Controller Firmware
Upgrade firmware on multiple storage subsystems concurrently.
Note: You MUST use this option in the Enterprise Management Window (EMW) to upgrade a storage subsystem from pre-07.xx.xx.xx controller firmware to 07.xx.xx.xx or later.You cannot use the Download Controller Firmware option in the Subsystem Management Window to complete this specific upgrade task.

Accessibility

Inherit System Settings
Inherit system settings for color and font allows the IBM DS Storage Manager 10 software to use settings you define through your operating system.

Fig: Array Management console.

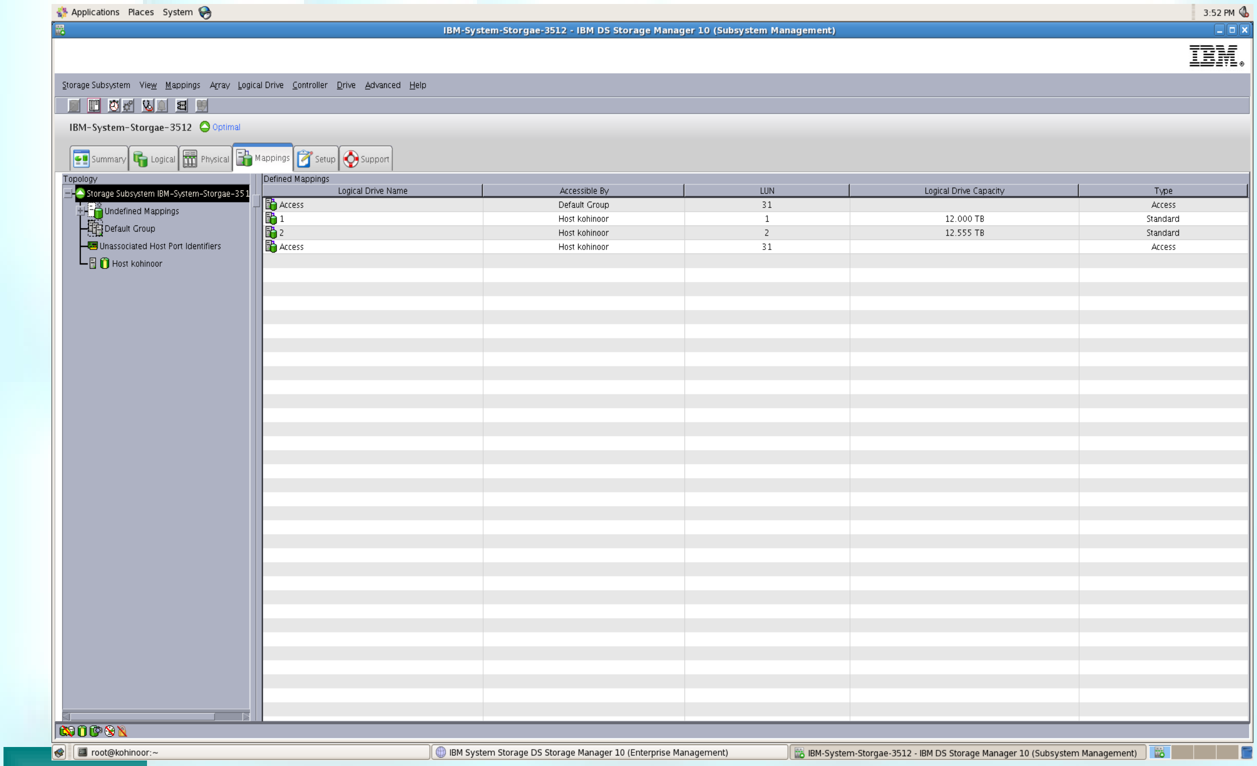

Applications Places System
3:52 PM
IBM-System-Storgae-3512 - IBM DS Storage Manager 10 (Subsystem Management)
IBM
Storage Subsystem View Mappings Array Logical Drive Controller Drive Advanced Help
IBM-System-Storgae-3512 Optimal
Summary Logical Physical Mappings Setup Support
Logical
Storage Subsystem IBM-System-Storgae-3512
IBM-DAS (RAID 5) (24.556 TB)
1 (12.000 TB)
2 (12.555 TB)
3 (500.000 MB)
Free Capacity (328.148 MB)
Properties
root@kohinoor:~
IBM System Storage DS Storage Manager 10 (Enterprise Management)
IBM-System-Storgae-3512 - IBM DS Storage Manager 10 (Subsystem Management)

Storage Subsystem "IBM-System-Storgae-3512"

View Complete Storage Subsystem Profile

```
Summary Profile:
Controller redundancy mode:     Simplex (single controller)
Number of controllers:          1

High performance tier controllers: Disabled

Number of arrays:               1

RAID 6:                         Enabled

Total number of logical drives used:    4
   Number of standard logical drives:   3
   Number of access logical drives:     1
Total number of logical drives allowed: 512

Drive Limit Management:
   Number of drive slots discovered: 12
   Number of drive slots allowed:    96

FlashCopy Logical Drives:                            Enabled
   Number of flashcopies used:                       0
   Number of flashcopies allowed:                    2
   Number of flashcopies allowed per base logical drive: 2

Solid State Disk Support:    Disabled
   Number of drives used:    0
   Number of drives allowed: 0

Enhanced Remote Mirroring (ERM): Disabled/Deactivated
   Number of mirrors used:       0
   Number of mirrors allowed:    0

VolumeCopy:                Disabled
   Number of copies used:  0
   Number of copies allowed: 0

Number of drives:          12
```

Fig: Logical Volume view of the Storage.


Applications Places System
3:52 PM
IBM-System-Storgae-3512 - IBM DS Storage Manager 10 (Subsystem Management)
IBM
Storage Subsystem View Mappings Array Logical Drive Controller Drive Advanced Help
IBM-System-Storgae-3512 Optimal
Summary Logical Physical Mappings Setup Support
Topology
Storage Subsystem IBM-System-Storgae-351
Undefined Mappings
Default Group
Unassociated Host Port Identifiers
Host kohinoor
Defined Mappings
root@kohinoor:~
IBM System Storage DS Storage Manager 10 (Enterprise Management)
IBM-System-Storgae-3512 - IBM DS Storage Manager 10 (Subsystem Management)

Logical Drive Name	Accessible By	LUN	Logical Drive Capacity	Type
Access	Default Group	31		Access
1	Host kohinoor	1	12.000 TB	Standard
2	Host kohinoor	2	12.555 TB	Standard
Access	Host kohinoor	31		Access

Fig: Logical volume mapping to Host.

3.4. Operating System - CentOS:

An operating system is software, consisting of programs and data that runs on computers manages computer hardware resources, and provides common services for execution of various application software. Operating system is the most important type of system software in a computer system. Without an operating system, a user cannot run an application program on their computer, unless the application program is self booting.

For hardware functions such as input and output and memory allocation, the operating system acts as an intermediary between application programs and the computer hardware, although the application code is usually executed directly by the hardware and will frequently call the OS or be interrupted by it. Operating systems are found on almost any device that contains a computer—from cellular phones and video game consoles to supercomputers and web servers.

Examples of popular modern operating systems are: BSD, Linux, Mac OS X, Microsoft Windows and UNIX.

Linux refers to the family of Unix-like computer operating systems using the Linux kernel. Linux can be installed on a wide variety of computer hardware, ranging from mobile phones, tablet computers, routers, and video game consoles, to mainframes and supercomputers. Linux is a leading server operating system, and runs the 10 fastest supercomputers in the world.

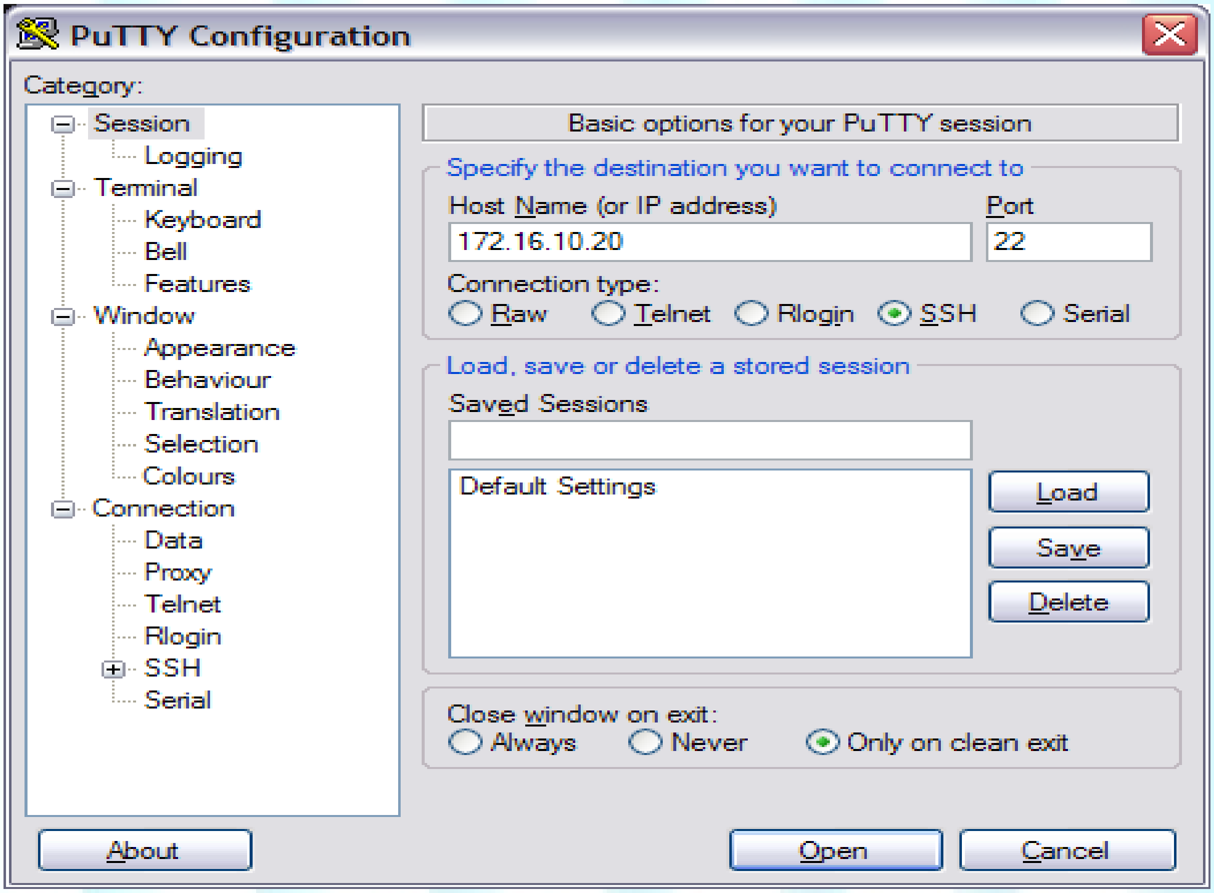
The development of Linux is one of the most prominent examples of free and open source software collaboration; typically all the underlying source code can be used, freely modified, and redistributed, both commercially and non-commercially, by anyone under licenses such as the GNU General Public License. Typically Linux is packaged in a format known as a Linux distribution for desktop and server use. Some popular mainstream Linux distributions include Debian (and its derivatives such as Ubuntu), Fedora and openSUSE. Linux distributions include the Linux kernel and supporting utilities and libraries to fulfill the distribution's intended use.

3.5. Cluster Management

Login from Windows Machine

Step1:
Get the latest version of putty

Step2:
Run putty and try to ssh connection to <cluster public IP Address>



Host Name (or IP address): 172.16.10.20

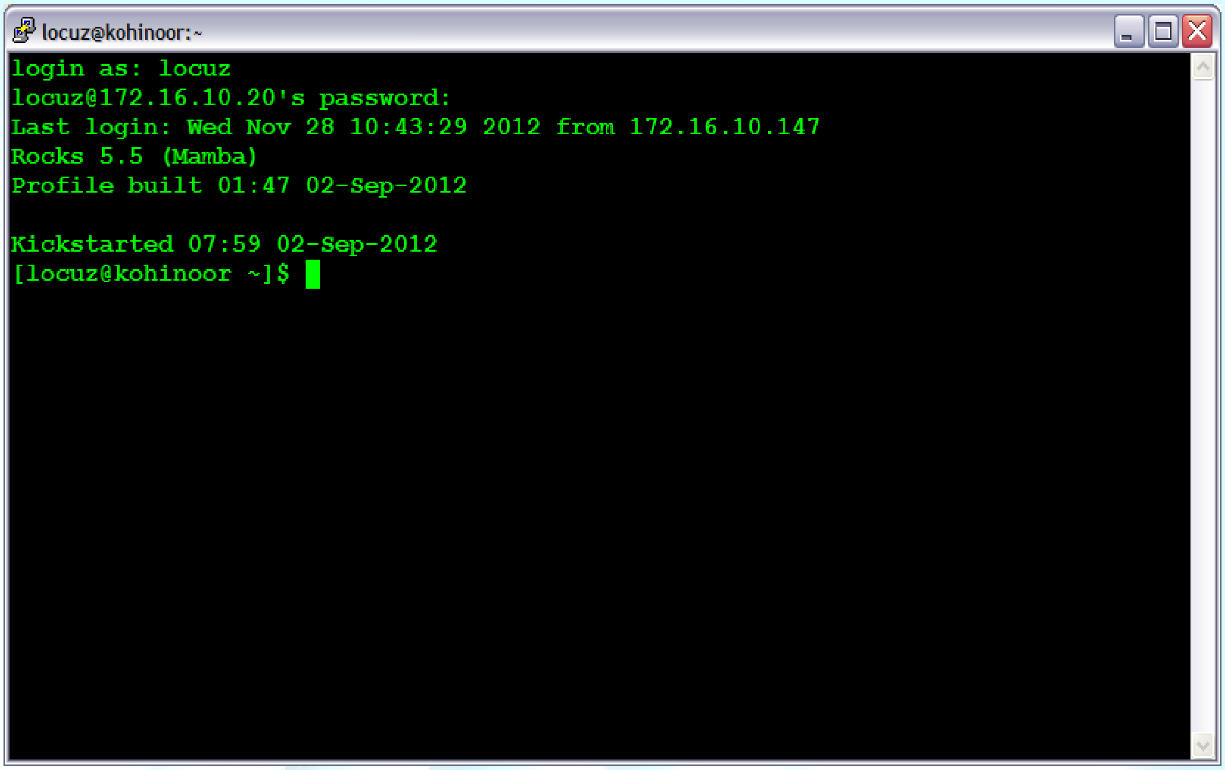
Port: 22

Connection type: ○ Raw ○ Telnet ○ Rlogin ● SSH ○ Serial

Saved Sessions:

Default Settings

Close window on exit: ○ Always ○ Never ● Only on clean exit



```
login as: locuz
locuz@172.16.10.20's password:
Last login: Wed Nov 28 10:43:29 2012 from 172.16.10.147
Rocks 5.5 (Mamba)
Profile built 01:47 02-Sep-2012

Kickstarted 07:59 02-Sep-2012
[locuz@kohinoor ~]$
```

Logged in as a user locuz

Login from Linux machine

[root@localhost ~] ssh locuz@172.16.10.20
Password:

[locuz@kohinoor ~]$

Creating User account into the Kohinoor cluster

User Creation:

Create a user account and propagate the information to the compute nodes with:

```
# useradd <username>
# passwd <username>
New password:
Re-enter password:
```

It creates a user's home directory at location **/export/home/$USER**

```
# rocks sync users
```

Update all user-related files (e.g., /etc/passwd, /etc/shadow, etc.) on all known hosts. Also, restart autofs on all known hosts.

User deletion:

```
# userdel <username>
```

Then run the

```
# rocks sync users
```

Update all user-related files (e.g., /etc/passwd, /etc/shadow, etc.)

Copy a file or directory of every compute node:

```
$ rocks iterate host compute "scp <file> %:/tmp/"
```

Copies file to the /tmp directory of every compute node

```
$ rocks iterate host compute "scp -r <directory> %:/tmp/"
```

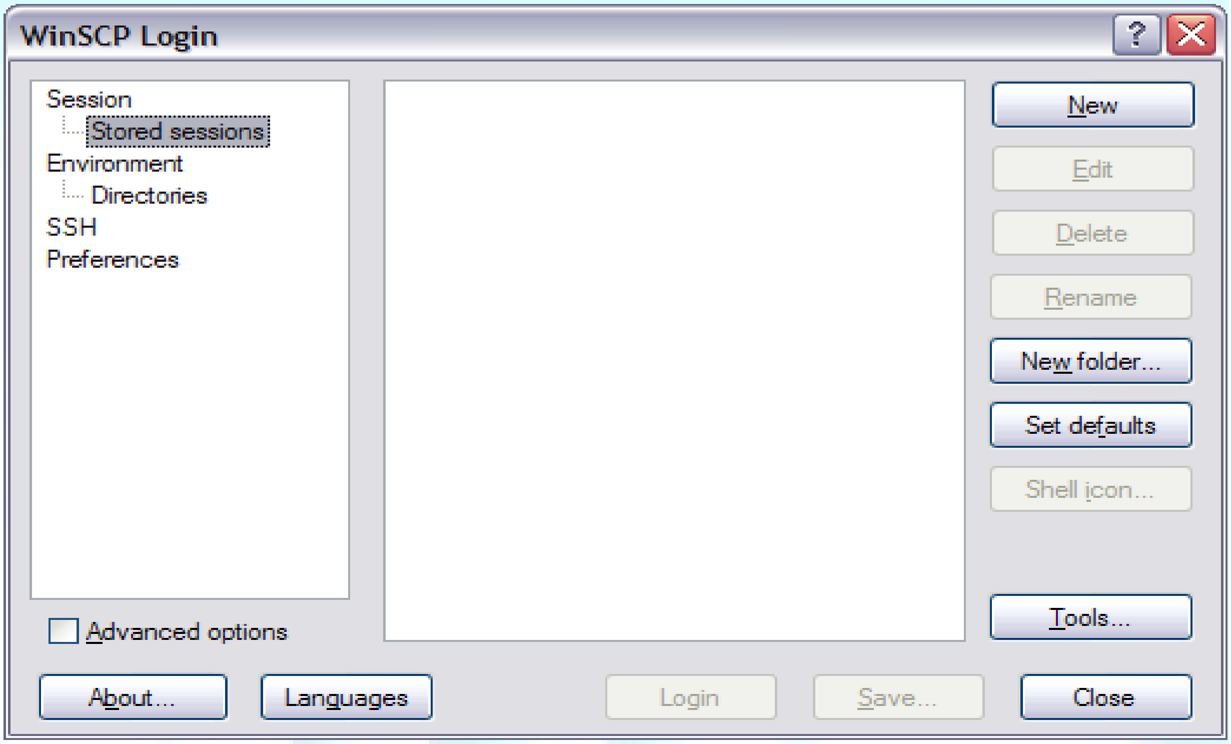
Copy a directory to the /tmp directory of every compute node

Copy a file to defined compute node:

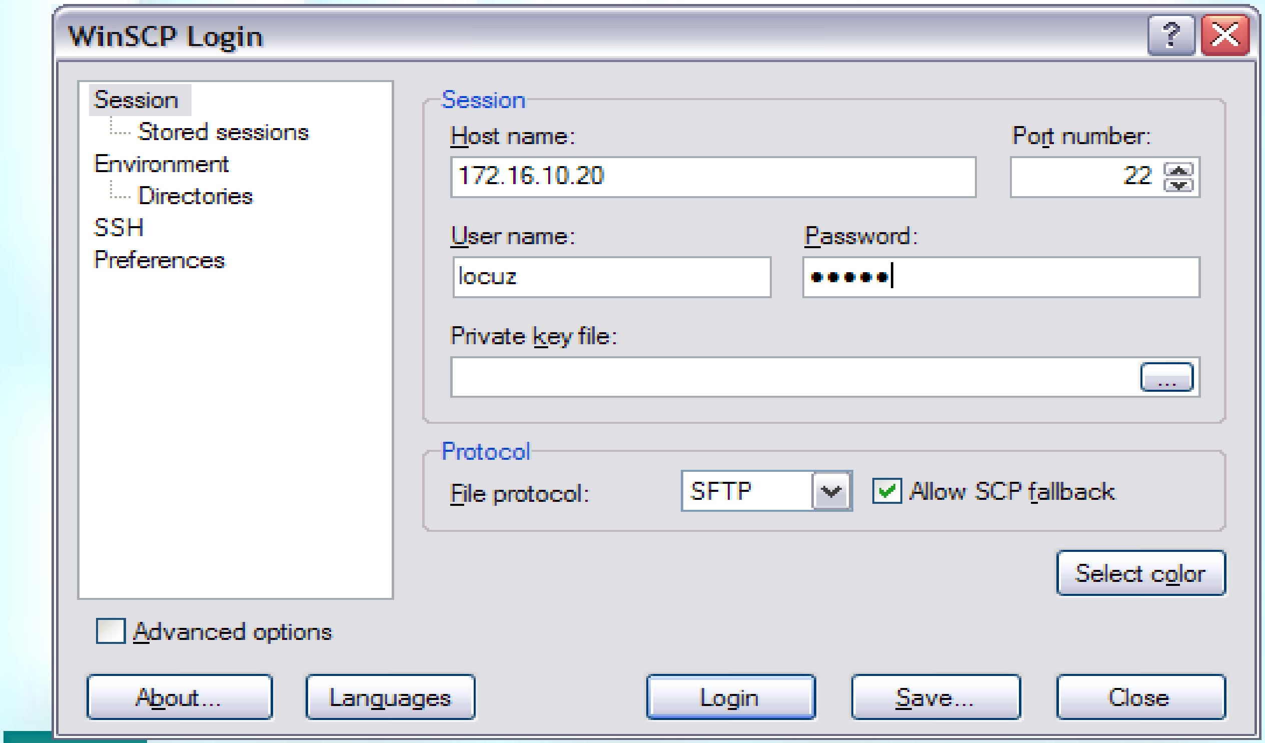
```
$ scp <filename> <compute node name>:/tmp

$ scp -r <directory> <compute node name>:/tmp
```

Copy a data from end-user Windows machine to cluster

Step 1:
Install and start WinSCP, then following screen is shown. Click 'New' button.



Step 2:
Following screen is shown. Input information’s to login like below.



WinSCP Login

Session

Host name: 172.16.10.20

Port number: 22

User name: locuz

Password: •••••

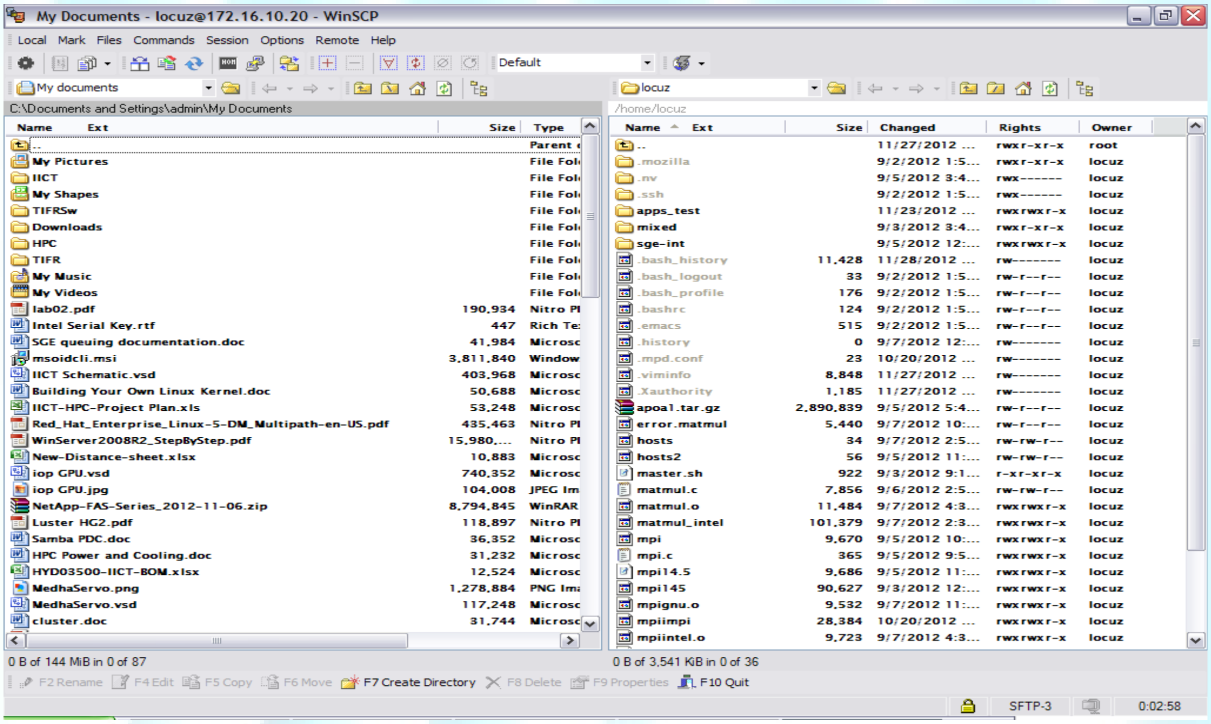
Private key file:

Protocol

File protocol: SFTP

☑ Allow SCP fallback

Step 3:
It’s possible to upload or download files



C:\Documents and Settings\admin\My Documents

Name Ext	Size	Type
..		Parent d
My Pictures		File Fol
IICT		File Fol
My Shapes		File Fol
TIFRSw		File Fol
Downloads		File Fol
HPC		File Fol
TIFR		File Fol
My Music		File Fol
My Videos		File Fol
lab02.pdf	190,934	Nitro PI
Intel Serial Key.rtf	447	Rich Te:
SGE queuing documentation.doc	41,984	Microsc
msoidcli.msi	3,811,840	Window
IICT Schematic.vsd	403,968	Microsc
Building Your Own Linux Kernel.doc	50,688	Microsc
IICT-HPC-Project Plan.xls	53,248	Microsc
Red_Hat_Enterprise_Linux-5-DM_Multipath-en-US.pdf	435,463	Nitro PI
WinServer2008R2_StepByStep.pdf	15,980,...	Nitro PI
New-Distance-sheet.xlsx	10,883	Microsc
iop GPU.vsd	740,352	Microsc
iop GPU.jpg	104,008	JPEG Im
NetApp-FAS-Series_2012-11-06.zip	8,794,845	WinRAR
Luster HG2.pdf	118,897	Nitro PI
Samba PDC.doc	36,352	Microsc
HPC Power and Cooling.doc	31,232	Microsc
HYD03500-IICT-BOM.xlsx	12,524	Microsc
MedhaServo.png	1,278,884	PNG Ima
MedhaServo.vsd	117,248	Microsc
cluster.doc	31,744	Microsc

0 B of 144 MiB in 0 of 87

/home/locuz

Name Ext	Size	Changed	Rights	Owner
..		11/27/2012 ...	rwxr-xr-x	root
.mozilla		9/2/2012 1:5...	rwxr-xr-x	locuz
.nv		9/5/2012 3:4...	rwx------	locuz
.ssh		9/2/2012 1:5...	rwx------	locuz
apps_test		11/23/2012 ...	rwxrwxr-x	locuz
mixed		9/3/2012 3:4...	rwxr-xr-x	locuz
sge-int		9/5/2012 12:...	rwxrwxr-x	locuz
.bash_history	11,428	11/28/2012 ...	rw-------	locuz
.bash_logout	33	9/2/2012 1:5...	rw-r--r--	locuz
.bash_profile	176	9/2/2012 1:5...	rw-r--r--	locuz
.bashrc	124	9/2/2012 1:5...	rw-r--r--	locuz
.emacs	515	9/2/2012 1:5...	rw-r--r--	locuz
.history	0	9/7/2012 12:...	rw-------	locuz
.mpd.conf	23	10/20/2012 ...	rw-------	locuz
.viminfo	8,848	11/27/2012 ...	rw-------	locuz
.Xauthority	1,185	11/27/2012 ...	rw-------	locuz
apoa1.tar.gz	2,890,839	9/5/2012 5:4...	rw-r--r--	locuz
error.matmul	5,440	9/7/2012 10:...	rw-r--r--	locuz
hosts	34	9/7/2012 2:5...	rw-rw-r--	locuz
hosts2	56	9/5/2012 11:...	rw-rw-r--	locuz
master.sh	922	9/3/2012 9:1...	r-xr-xr-x	locuz
matmul.c	7,856	9/6/2012 2:5...	rw-rw-r--	locuz
matmul.o	11,484	9/7/2012 4:3...	rwxrwxr-x	locuz
matmul_intel	101,379	9/7/2012 2:3...	rwxrwxr-x	locuz
mpi	9,670	9/5/2012 10:...	rwxrwxr-x	locuz
mpi.c	365	9/5/2012 9:5...	rwxrwxr-x	locuz
mpi14.5	9,686	9/5/2012 11:...	rwxrwxr-x	locuz
mpi145	90,627	9/3/2012 12:...	rwxrwxr-x	locuz
mpignu.o	9,532	9/7/2012 11:...	rwxrwxr-x	locuz
mpiimpi	28,384	10/20/2012 ...	rwxrwxr-x	locuz
mpiintel.o	9,723	9/7/2012 4:3...	rwxrwxr-x	locuz

0 B of 3,541 KiB in 0 of 36

Copy a data from end-user Linux machine to cluster

```
[root@localhost ~] scp <filename> locuz@172.16.10.20
```

Coping a file into user locuz home directory

```
[root@localhost ~] scp –r <directory> locuz@172.16.10.20
```

Coping a directory into user locus home directory

Rocks run host:
Used to run any command on compute node of the cluster

```
$ rocks run host “<command>”
```

Run the particular command on all nodes

```
$ rocks run host -n <node name> "<command>"
```

Run the particular command on specific node

3.6. Software – Compilers, Libraries, Visualization & Applications

Compilers:

a. GNU compilers

C	=	/usr/bin/gcc
C++	=	/usr/bin/g++
FORTRAN	=	/usr/bin/gfortran, /usr/bin/f95

b. INTEL compilers

C	=	/export/data/intel/Compiler/11.1/080/bin/intel64/icc
C++	=	/export/data/intel/Compiler/11.1/080/bin/intel64/icpc
FORTRAN	=	/export/data/intel/Compiler/11.1/080/bin/intel64/ifort

c. PGI compilers

C	=	/export/data/pgi/linux86-64/12.8/bin/pgcc
C++	=	/export/data/pgi/linux86-64/12.8/bin/{pgCC,pgc++}
FORTRAN	=	export/data/pgi/linux86-64/12.8/bin/{pgf77, pgf90, pgf95}

d. GPU NVIDIA CUDA compilers

C	=	/usr/local/cuda/bin/nvcc [NVIDIA]
C++	=	/export/data/pgi/linux86-64/12.8/bin/pgc++ [PGI]
FORTRAN	=	/export/data/pgi/linux86-64/12.8/bin/pgfortran [PGI]

e. MPI (Parallel) compilers

mpicc	=	/export/data/mpi/openmpi/1.4.5/intel/bin/mpicc
mpic++	=	/export/data/mpi/openmpi/1.4.5/intel/bin/mpic++

mpif77 = /export/data/mpi/openmpi/1.4.5/intel/bin/mpif77

mpif90 = /export/data/mpi/openmpi/1.4.5/intel/bin/mpif90

Libraries:

a. INTEL Math Kernel Library (MKL) (Lapack, Blas, Scalapack, Blacs)

Location (MKLROOT) = /export/data/intel/Compilers/11.1/080/mkl/ /lib/em64t

Linking file = -L$(MKLROOT)/lib/intel64 -lmkl_scalapack_ilp64 -lmkl_intel_ilp64 -lmkl_sequential -lmkl_core -lmkl_blacs_intelmpi_ilp64 -lpthread -lm

For more information, please refer following web link:
http://software.intel.com/sites/products/mkl/MKL_Link_Line_Advisor.html

b. SCIPY,NUMPY

SCIPY = /usr/lib64/python2.4/site-packages/scipy

NUMPY = /export/data/apps/numpy/1.6.2/intel

c. GSL

Location = /export/data/libs/gsl/1.15/intel

Executable file = /export/data/libs/gsl/1.15/intel/bin/{gsl-config, gsl-histogram, gsl-randist}

Visualization:

a. GPUPLOT

Location = /usr

Executable file = /usr/bin/gnuplot

b. XMGRACE

Location = /export/data/apps/grace/5.1.22/int-fft-net/grace/

Executable file = /export/data/apps/grace/5.1.22/int-fft-net/grace/bin/xmgrace

c. PYMOL

d. JMOL

Location = /export/data/apps/jmol/13.0.2

Executable file = /export/data/apps/jmol/13.0.2/jmol.sh

e. VMD

Location = /export/data/apps/vmd/1.8.6

Executable file = /export/data/apps/vmd/1.8.6/LINUXAMD64/vmd_LINUXAMD64

Applications:

List of Application

Sl.No	Application Name	CPU	GPU
A	LAMMPS	Yes	Yes
B	NAMD	Yes	Yes
C	GROMACS	Yes	Yes
D	CPMD	Yes	NA
E	QUANTUM ESPRESSO	Yes	NA
F	SIESTA	Yes	NA
G	ABINIT	Yes	NA
H	RUMD	NA	Yes
I	HOOMD	Yes	Yes
J	VASP		

A. LAMMPS

CPU:

Location	=	/export/data/apps/lammps-cpu
Executable file	=	/export/data/apps/lammps-cpu/30Aug12/bin/lmp_openmpi

GPU:

Location	=	/export/data/apps/lammps-cuda
Executable file	=	/export/data/apps/lammps-cuda/bin/lmp_cuda

B. NAMD

CPU:

Location	=	/export/data/apps/NAMD_2.9_Linux-x86_64-ibverbs
Executable file	=	/export/data/apps/NAMD_2.9_Linux-x86_64-ibverbs/namd2

GPU:

Location	=	/export/data/apps/NAMD_2.9_Linux-x86_64-multicore-CUDA
Executable file	=	/export/data/apps/NAMD_2.9_Linux-x86_64-multicore-CUDA/namd2

C. GROMACS

CPU:

Location	=	/export/data/apps/gromacs
Executable file	=	/export/data/apps/gromacs/4.5.5/intel/bin/mdrun_mpi

GPU:

Location	=	/export/data/apps/gromacs-gpu

Executable file = /export/data/apps/gromacs-gpu/mdrun-openmm

D. CPMD

CPU:

Location = /export/data/apps/cpmd

Executable file = /export/data/apps/cpmd/3.15.3/intel-ompi/cpmd.x

E. QUANTUM ESPRESSO

CPU:

Location = /export/data/apps/q-espresso

Executable file = /export/data/apps/q-espresso/5.0/intel-ompi/bin/pw.x

F. SISETA

CPU:

Location = /export/data/apps/siesta

Executable file = /export/data/apps/siesta/3.1/intel-ompi/bin/siesta

G. ABINIT

CPU:

Location = /export/data/apps/abinit

Executable file = /export/data/apps/abinit/6.12.3/intel-ompi/bin/abinit

H. RUMD

GPU:

Location=

Executable file=

I. HOOMD

CPU:

Location	=	/usr/bin
Executable file	=	/usr/bin/hoomd

GPU:

Location	=	/usr/bin
Executable file	=	/usr/bin/hoomd

J. VASP

3.7. Scheduler & Distributed Resource Manager (SGE)

Oracle Grid Engine, previously known as Sun Grid Engine (SGE) is an open source batch-queuing system, developed and supported by Sun Microsystems. Sun once also sold a commercial product based on SGE, known as N1 Grid Engine (N1GE).

SGE is typically used on a computer farm or high-performance computing (HPC) cluster and is responsible for accepting, scheduling, dispatching, and managing the remote and distributed execution of large numbers of standalone, parallel or interactive user jobs. It also manages and schedules the allocation of distributed resources such as processors, memory, disk space, and software licenses.

Features new in version:

- Advance reservation
- Array job interdependencies
- Rule-based Resource Quota control
- Enhanced remote execution (without using external rshd/rlogind/sshd processes)
- Multi-clustering
- Daemons managed by the Service Management Facility on Solaris

- Pseudo TTY (pty) support for interactive jobs
- Job Submission Verifier (client-side and server-side job verification)
- GUI Installer and SGE Inspect
- Topology-aware scheduling and thread binding
- Hadoop integration, Amazon EC2 integration for cloud computing

Other features of SGE include:

- Multiple advanced scheduling algorithms allow powerful policy-based resource allocation Cluster queues
- Job and scheduler fault tolerance - Grid Engine continues to operate as long as there is one or more hosts available
- Job checkpointing
- Job arrays and job tasks
- DRMAA (Job API)
- Resource reservation
- XML status reporting (qstat and qhost), and the xml-qstat web interface
- Parallel jobs (MPI, PVM, OpenMP), and scalable parallel job startup with qrsh[10]
- Usage accounting
- Accounting and Reporting COnsole (ARCO)
- parallel make: distmake, dmake (Sun Studio), and SGE's own qmake
- FLEXlm integration and multi-cluster software license management with LicenseJuggler

Use the qsub Command to Submit a Job:

The **qsub** command is used to submit jobs to SGE. The syntax of the qsub command is:

```
$ qsub [-cwd] [-v SOME_VAR] [-o path] [-e path] \
     [-M mail_address][-m mail_options] [-l resources] script
```

Where:

-cwd

Directs SGE to run the job in the same directory from which we submitted it. Alternatively, we can specify this flag in the SGE command file for the job.

-v *SOME_VAR*

Passes environment variable *SOME_VAR* to the job. Alternatively, we can specify this flag in the SGE command file for the job.

-o *path*

Redirects stdout from the SGE script. The default is home directory. Specify /dev/null to disgard SGE messages. Alternatively, we can specify this flag in the SGE command file for the job.

-e *path*

Redirects stderr from the SGE script. The default is home directory. Specify /dev/null to disgard SGE error messages. Alternatively, we can specify this flag in the SGE command file for the job.

-M *mail_address*

where *mail_address* is user's email address. It is always *login_id*@mail on Hoffman2.

-m *mail_options*

Specifies the circumstances under which mail is to be sent to the job owner defined by -M option. For example options "bea" mean mail is sent at the begining, end, and at abort time (if it happens) of the job. Option "n" means no mail will be sent.

-l *resources*

Specifies a list of resouces required for the job, for example memory and time per core:

-l h_data=1024M,h_rt=24:00:00

script

Either the SGE command file or the script that starts up the job.

The qsub command line switches and options can also be used as active comments or embedded directives in an SGE command file that we submit with the qsub command. Advantages of this approach are: we have a record of what options were used to run our job; we can easily resubmit jobs; and we can use one command file as the basis for creating other similar command files. For example, if the file myjob.cmd contains:

```
#!/bin/csh
/path/to/executable
```

and the qsub command used to submit it is:

```
$ qsub -cwd -o path -M login_id@mail -m bea \
               -l h_data=1024M,h_rt=24:00:00 myjob.cmd
```

then the same result could be achieved by adding the following lines to the myjob.cmd file before the */path/to/executable* line:

```
#$ -cwd
#$ -o path
#$ -M login_id@mail
#$ -m bea
#$ -l h_data=1024M,h_rt=24:00:00
```

and submitting the myjob.cmd script with:

```
$ qsub myjob.cmd
```

After submitting a job with qsub, SGE will respond with something like:

```
Your job 624556 ("myjob.cmd") has been submitted
```

where 624556 is the job number assigned by SGE to the job.

Use the qstat Command to Determine the Status of a Job:

The **qstat** command displays information about the jobs in the SGE queues, both running and waiting to run. The syntax of the qstat command is:

```
$ qstat [-f] [-j job_number] [-U login_id] [-u login_id]
```

where:

(qstat alone with no arguments)
Displays a list of all running and waiting jobs.

-f
Displays summary information on each queue as well as the job list.

-j *job_number*
Displays the status of the job whose job number is *job_number*

-U *login_id*
Displays a list of running and waiting jobs for those queues which *login_id* can access. Or use the **groupjobs** script for this information; enter *groupjobs -help* for usage information.

-u *login_id*
Displays a list of *login_id* 's running and waiting jobs. Or use the **myjobs** script for this information for our own login_id.

Use the qhost Command to Display Node Information:

The **qhost** command displays information about compute nodes: their architectures, number of processors, load, etc. The syntax of the qhost command is:

```
$ qhost [-j] [-q]
```

where:

(qhost alone with no arguments)
Displays a table of information about the compute nodes.

-j
Adds information about the specific jobs that are running on each compute node.

-q
Shows the queues each compute node accepts.

Use the qdel Command to Cancel a Job:

The **qdel** command is used to cancel a job either while it is waiting to execute or while it is running. The syntax of the qdel command is:

```
$ qdel job_number
```

If a running job does not get cancelled right away, enter:

```
$ qdel -f job_number
```

to force it to be cancelled. Jobs in the "dr" state (disabled running) cannot be cancelled by the job owner. They must be cancelled by a system administrator. "dr" state jobs usually indicate a system hardware problem.

Queue list

A. **gpu.q** **--** This queue is for gpu/cuda jobs, with no time limit.

B. **long.q** **--** This queue is for long parallel jobs, with 15 days time limit.

C. **short.q** **--** This queue is for short parallel jobs, with 5 days time limit.

D. **serial.q** **--** This queue is for serial jobs (single core), with no time limit.

a. ABINIT

Version=6.12.3
PATH=/export/data/apps/abinit/6.12.3

Job Script

The following job script is adequate for running of ABINIT application

```
$vi abinit_cpu_sge.sh
#!/bin/bash
#$ -N ABINIT
#$ -cwd
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16

/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np
$NSLOTS  /export/data/apps/abinit/6.12.3/intel-ompi/bin/abinit
```

Job Submission

```
$qsub abinit_cpu_sge.sh
```

b. CPMD

Version=3.15.3
PATH=/export/data/apps/cpmd/3.15.3

Job Script

```
#!/bin/bash
#$ -N CPMD
#$ -cwd
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16

/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np
$NSLOTS  /export/data/apps/cpmd/3.15.3/intel-ompi/cpmd.x
```

Job Submission

```
$qsub cpmd_cpu_sge.sh
```

c. GROMACS

CPU
Version=4.5.5
PATH=/export/data/apps/gromacs/4.5.5

Job Scripts

```
#!/bin/bash
#$ -N Gromacs
#$ -cwd
#$ -S /bin/bash
#$ -q serial.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID

/export/data/apps/gromacs/4.5.5/intel/bin/grompp_mpi
/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np $NSLOTS
/export/data/apps/gromacs/4.5.5/intel/bin/mdrun_mpi
```

Job Submission

```
$qsub gromacs_cpu_sge.sh
```

GPU
Version=
PATH=/export/data/apps/gromacs-gpu

Job scripts

```
#!/bin/bash
#$ -N GMX-GPU
#$ -cwd
#$ -S /bin/bash
#$ -q gpu.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -l gpu=1

# /export/data/apps/gromacs/4.5.5/intel-ompi/bin/grompp_mpi
#$ -v LD_LIBRARY_PATH=/export/data/apps/gromacs-
gpu:/export/data/apps/gromacs-gpu/cuda23/lib64
#$ -v OPENMM_PLUGIN_DIR=/export/data/apps/gromacs-gpu
#$ -v OPENMM_PLATFORM=Cuda,CudaDevice=1
export LD_LIBRARY_PATH=/export/data/apps/gromacs-
gpu:/export/data/apps/gromacs-gpu/cuda23/lib64
export OPENMM_PLUGIN_DIR=/export/data/apps/gromacs-gpu
export OPENMM_PLATFORM=Cuda,CudaDevice=0
/export/data/apps/gromacs-gpu/mdrun-openmm
```

Job Submission

```
$qsub gromacs_gpu_sge.sh
```

d. HOOMD

CPU
Version=0.11.0
PATH=

Job script

```
#!/bin/bash
#$ -N hoomd-cpu
#$ -cwd
#$ -S /bin/bash
#$ -q serial.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -v OMP_NUM_THREADS=1

export OMP_NUM_THREADS=1

/usr/bin/hoomd lj_liquid_bmark.hoomd
```

Job submission

```
$qsub hoomd_cpu_serial_sge.sh
```

GPU
Version=0.11.0
PATH=

Job script

```
#!/bin/bash
#$ -N hoomdgpu
#$ -cwd
#$ -S /bin/bash
#$ -q gpu.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 1
#$ -l gpu=1
#$ -v OMP_NUM_THREADS=1

export OMP_NUM_THREADS=1

/usr/bin/hoomd lj_liquid_bmark.hoomd
```

Job submission

```
$qsub hoomd_gpu_sge.sh
```

e. LAMMPS

CPU
Version=
PATH= /export/data/apps/lammps-cpu

Job scripts

```
#!/bin/bash
#$ -N LAMMPS-CPU
#$ -cwd
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16

/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np $NSLOTS
/export/data/apps/lammps-cpu/30Aug12/bin/lmp_openmpi
```

Job Submission

```
$qsub lammps_cpu_sge.sh
```

GPU
Version=
PATH= /export/data/apps/lammps-cuda

Job scripts

```
#!/bin/bash
#$ -N Lammps-cuda
#$ -cwd
#$ -S /bin/bash
#$ -q gpu.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -l gpu=1

#$ -v LD_LIBRARY_PATH=/export/data/apps/gromacs-
gpu:/export/data/apps/gromacs-gpu/cuda23/lib64
export LD_LIBRARY_PATH=/export/data/apps/gromacs-
gpu:/export/data/apps/gromacs-gpu/cuda23/lib64
/export/data/mpi/openmpi/1.6.1/intel/bin/mpirun -np 1
/export/data/apps/lammps-cuda/bin/lmp_cuda  -sf cuda -v g 1 -v
x 16 -v y 16 -v z 16 -v t 100 < in.lj.cuda
```

Job Submission

```
$qsub lammps_gpu_sge.sh
```

f. NAMD

CPU
Version=2.9
PATH= /export/data/apps/NAMD_2.9_Linux-x86_64-ibverbs

Job script

```
#!/bin/bash
#$ -N Namd
#$ -cwd
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe mpi 32

nodefile=$TMPDIR/namd2.nodelist
echo group main > $nodefile
awk '{ for (i=0;i<$2;++i) {print "host",$1} }' $PE_HOSTFILE >>
$nodefile

cat $nodefile
dir=/export/data/apps/NAMD_2.9_Linux-x86_64-ibverbs
$dir/charmrun ++remote-shell ssh ++nodelist $nodefile +p$NSLOTS
$dir/namd2 apoa1.namd
```

Job Submission

```
$qsub namd_cpu_sge.sh
```

GPU
Version=2.9
PATH=/export/data/apps/NAMD_2.9_Linux-x86_64-multicore-CUDA

Job scripts

```
#!/bin/bash
#$ -N Namd-CUDA
#$ -cwd
#$ -S /bin/bash
#$ -q gpu.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -l gpu=1
#$ -v LD_LIBRARY_PATH=/export/data/apps/NAMD_2.9_Linux-x86_64-
multicore-CUDA:$LD_LIBRARY_PATH

export  LD_LIBRARY_PATH=/export/data/apps/NAMD_2.9_Linux-
x86_64-multicore-CUDA:$LD_LIBRARY_PATH
```

```
/export/data/apps/NAMD_2.9_Linux-x86_64-multicore-CUDA/namd2
+idlepoll  apoa1.namd
```

Job Submission

```
$qsub namd_gpu_sge.sh
```

g. QUANTUM ESPRESSO

Version=5.0
PATH= /export/data/apps/q-espresso/5.0

Job scripts

```
#!/bin/bash
#$ -N QEspresso
#$ -cwd
#$ -S /bin/bash
#$ -q long.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16

/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np $NSLOTS
/export/data/apps/q-espresso/5.0/intel-ompi/bin/pw.x –in input
file > file.out
```

Job Submission

```
$qsub qespresso_cpu_sge.sh
```

h. SIESTA

Version=3.1
PATH= /export/data/apps/siesta/3.1

Job script

```
#!/bin/bash
#$ -N SIESTA
#$ -cwd
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16

/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np
$NSLOTS  /export/data/apps/siesta/3.1/intel-ompi/bin/siesta
```

Job submission

```
$qsub siesta_cpu_sge.sh
```

3.8. Troubleshooting SGE

(a) Submitting Serial Job

Batch or serial jobs can be submitted to SGE in two ways.
Using SGE job submit scripts

This example executes sleep command via job submit script method.

Create a script as follow:
[root@kohinoor ~]# vi submit.sh

```
        #!/bin/bash
        #$ -N Serial-Job
        #$  -cwd
        #$  -S /bin/bash
        #$ -e err.$JOB_ID.$JOB_NAME
        #$ -o out.$JOB_ID.$JOB_NAME

        sleep 100
```

Entries which start with #$ will be treated as SGE options.

- #$ **-cwd** means to execute the job for the current working directory.

- #$ -**S /bin/bash** specifies the interpreting shell for this job to be the Bash shell.

- #$ -N <job name> : The name to given to this job

- #$ -e <file name> : Mention the name of the file to store the errors

- #$ -o <file name> : Mention the name of the file to store the output

- #$ -q <queue name> : Mention the name of the queue

To submit this serial job script, you should use the **qsub** command.

```
[root@kohinoor~]# qsub submit.sh
your job 29 ("submit.sh") has been submitted
```

(b) Submitting Parallel Job

Using job submit script:

```
# cd ~
# vi test/mpi-ring.qsub
[root@  ~]# vi submit.sh

        #!/bin/bash
        #$ -N Parallel-Job
        #$  -cwd
        #$  -S /bin/bash
        #$ -e err.$JOB_ID.$JOB_NAME
        #$ -o out.$JOB_ID.$JOB_NAME
        #$ -q all.q
        #$ -pe orte 8
        /opt/mpi/openmpi/1.3.3/intel/bin/mpirun -np $NSLOTS ./a.out >
        outputfile
```

To submit the job:

```
$ qsub submit.sh
```

(c) Knowing the status of job

```
[root@Kohinoor~]# qstat
```

[root@kohinoor ~]# **qstat -j N**   N is the job id.

(d) Killing a Job

# qdel <jobid>

jobid is the pid of the job submitted which can be found when you use the qstat command.

Qhost

qhost shows the current status of the available Grid Engine hosts, queues and the jobs associated with the queues. Selection options allow you to get information about specific hosts, queues, jobs or users. Without any option qhost will display a list of all hosts without queue or job information.

```
[root@kohinoor ~]# qhost
```

Note: The scripts for running different applications under Sun Grid Engine, are kept in /JOB_SCRIPTS of the master node. Copy the scripts to your working directory. Edit the script with number of slots (for parallel jobs) and input file parameters and number of slots to use.

3.9. Monitoring Tool – Ganglia

Ganglia is a scalable distributed system monitor tool for high-performance computing systems such as clusters and grids. It allows the user to remotely view live or historical statistics (such as CPU load averages or network utilization) for all machines that are being monitored.

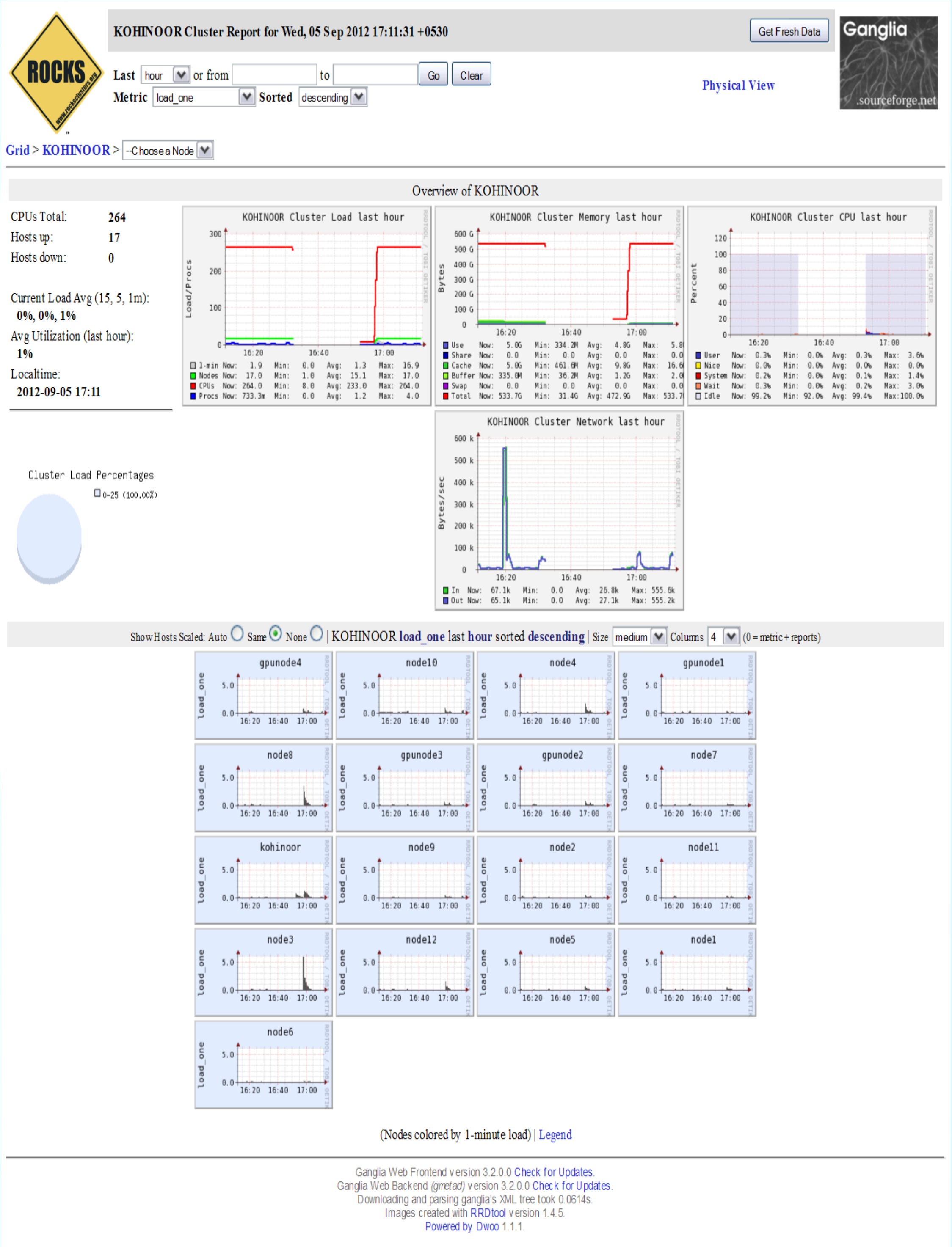
There are three services are mandatory for Ganglia. At server, httpd, gmetad and gmond, and at client, gmond only. If user wants to restart these services, he has to login as root, and restart three services at master node and one at every compute nodes:

```
# service httpd restart
# service gmetd restart
# service gmond restart
```

To open the web interface of Ganglia, type the following URL in browser:

http://172.16.10.20/ganglia

In Figure 3.13, there is a screenshot which give a brief picture of ganglia output:



KOHINOOR Cluster Report for Wed, 05 Sep 2012 17:11:31 +0530

Last hour or from to Go Clear

Metric load_one Sorted descending

Grid > KOHINOOR > --Choose a Node

Overview of KOHINOOR

CPUs Total: 264

Hosts up: 17

Hosts down: 0

Current Load Avg (15, 5, 1m):
0%, 0%, 1%

Avg Utilization (last hour):
1%

Localtime:
2012-09-05 17:11

```
□ 1-min Now:   1.9   Min: 0.0 Avg:   1.3 Max:  16.9
■ Nodes Now:  17.0   Min: 1.0 Avg:  15.1 Max:  17.0
■ CPUs  Now: 264.0   Min: 8.0 Avg: 233.0 Max: 264.0
■ Procs Now: 733.3m  Min: 0.0 Avg:   1.2 Max:   4.0
```

```
■ Use    Now:   5.0G Min: 334.2M Avg:   4.8G Max:   5.8
■ Share  Now:   0.0  Min:   0.0  Avg:   0.0  Max:   0.0
■ Cache  Now:   5.0G Min: 461.6M Avg:   9.8G Max:  16.6
■ Buffer Now: 335.0M Min:  36.2M Avg:   1.2G Max:   2.0
■ Swap   Now:   0.0  Min:   0.0  Avg:   0.0  Max:   0.0
■ Total  Now: 533.7G Min:  31.4G Avg: 472.9G Max: 533.7
```

```
■ User   Now:  0.3% Min:  0.0% Avg:  0.3% Max:  3.6%
■ Nice   Now:  0.0% Min:  0.0% Avg:  0.0% Max:  0.0%
■ System Now:  0.2% Min:  0.0% Avg:  0.1% Max:  1.4%
■ Wait   Now:  0.3% Min:  0.0% Avg:  0.2% Max:  3.0%
□ Idle   Now: 99.2% Min: 92.0% Avg: 99.4% Max:100.0%
```

```
■ In  Now: 67.1k Min: 0.0 Avg: 26.8k Max: 555.6k
■ Out Now: 65.1k Min: 0.0 Avg: 27.1k Max: 555.2k
```

Show Hosts Scaled: Auto ○ Same ● None ○ | KOHINOOR load_one last hour sorted descending | Size medium Columns 4 (0 = metric + reports)

(Nodes colored by 1-minute load) | Legend

Ganglia Web Frontend version 3.2.0.0 Check for Updates.
Ganglia Web Backend (gmetad) version 3.2.0.0 Check for Updates.
Downloading and parsing ganglia's XML tree took 0.0614s.
Images created with RRDtool version 1.4.5.
Powered by Dwoo 1.1.1.

Figure 3.13: Ganglia Monitoring Tool

3.10. System Management:

The integrated management module (IMM) consolidates the service processor functionality, Super I/O, video controller, and remote presence capabilities in a single chip on the server system board.

IMM features:

The IMM provides the following functions:

- Around-the-clock remote access and management of our server
- Remote management independent of the status of the managed server
- Remote control of hardware and operating systems
- Web-based management with standard Web browsers

IMM has the following features:

- Access to critical server settings
- Access to server vital product data (VPD)
- Advanced Predictive Failure Analysis (PFA) support
- Automatic notification and alerts
- Continuous health monitoring and control
- Choice of a dedicated or shared Ethernet connection
- Domain Name System (DNS) server support
- Dynamic Host Configuration Protocol (DHCP) support
- E-mail alerts
- Embedded Dynamic System Analysis (DSA)
- Enhanced user authority levels
- LAN over USB for in-band communications to the IMM
- Event logs that are time stamped, saved on the IMM, and can be attached to e-mail alerts
- Industry-standard interfaces and protocols
- OS watchdogs
- Remote configuration through Advanced Settings Utility (ASU)
- Remote firmware updating
- Remote power control
- Seamless remote accelerated graphics
- SecureWeb server user interface
- Serial over LAN
- Server console redirection
- Simple Network Management Protocol (SNMP) support
- User authentication using a secure connection to a Lightweight Directory Access

- Protocol (LDAP) server
- Remote presence, including the remote control of a server
- Operating-system failure screen capture and display through theWeb interface
- Remote disk, which enables the attachment of a diskette drive, CD/DVD drive, USB flash drive, or disk image to a server

The firmware included with this server is an implementation of Unified Extensible Firmware Interface (UEFI). It offers several features, such as UEFI 2.1 compliance, iSCSI compatibility, and enhanced reliability and service capabilities. The Setup utility provides server information, server setup, customization compatibility, and establishes the boot device order.

Web browser and operating-system requirements:

The IMMWeb interface requires the Java Plug-in 1.5 or later (for the remote presence feature) and one of the following Web browsers:

- Microsoft Internet Explorer version 6.0 or later with the latest Service Pack
- Mozilla Firefox version 1.5 or later

Accessing the IMM Web interface:

The IMM supports both static and Dynamic Host Configuration Protocol (DHCP) IP addressing. The default static IP address assigned to the IMM is 192.168.70.125. The IMM is initially configured to attempt to obtain an address from a DHCP server, and if it cannot, it uses the static IP address.

The IMM provides the choice of using a dedicated systems-management network connection or one that is shared with the server. The default connection for rack-mounted and tower servers is to use the dedicated systems-management network connector.

Logging in to the IMM:

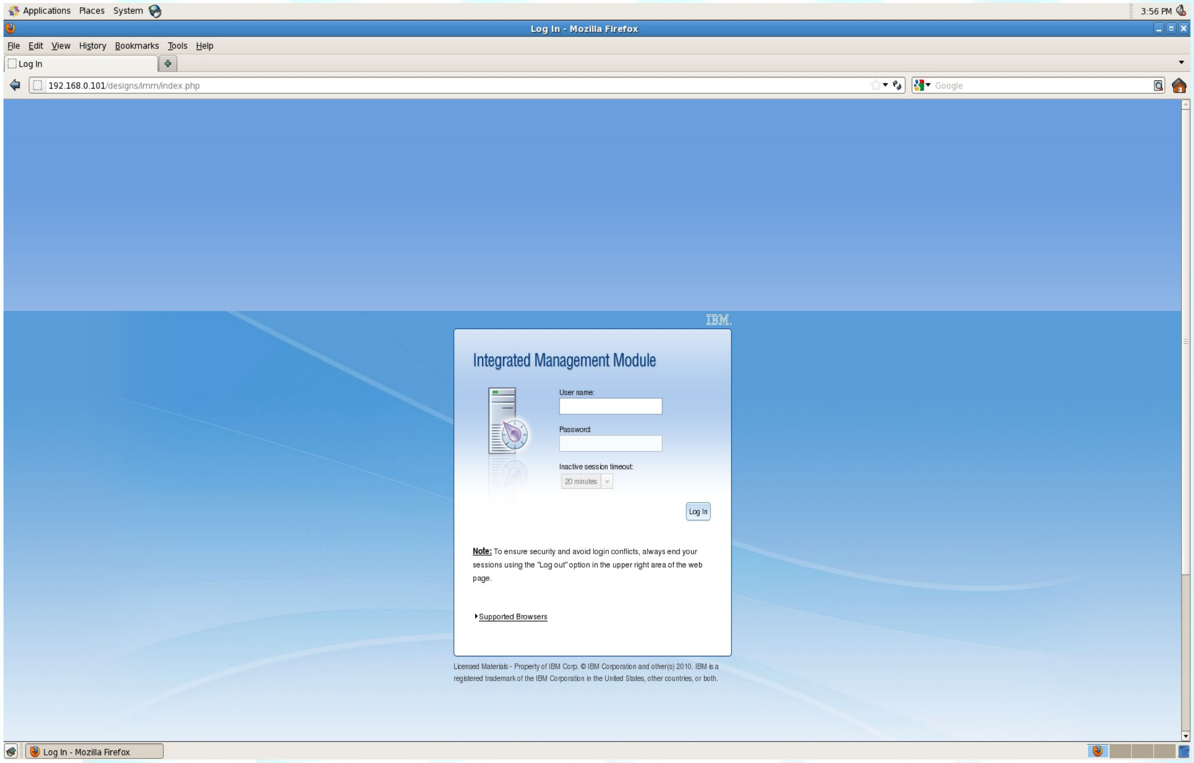
Important: The IMM is set initially with a user name of USERID and password of PASSW0RD (with a zero, not the letter O). This default user setting has Supervisor access.

Change this default password during our initial configuration for enhanced security.

To access the IMM through the IMM Web interface, complete the following steps:

1. Open a Web browser. In the address or URL field, type the IP address or host name of the IMM server to which we want to connect.

2. Type our user name and password in the IMM Login window. If we are using the IMM for the first time, we can obtain our user name and password from our system administrator. All login attempts are documented in the event log. Depending on how our system administrator configured the user ID, we might need to enter a new password.


Applications Places System
3:56 PM
Log In - Mozilla Firefox
File Edit View History Bookmarks Tools Help
Log In
192.168.0.101/designs/imm/index.php
Google
IBM.
Log In
Log In - Mozilla Firefox

Integrated Management Module

User name:

Password:

Inactive session timeout: 20 minutes

Note: To ensure security and avoid login conflicts, always end your sessions using the "Log out" option in the upper right area of the web page.

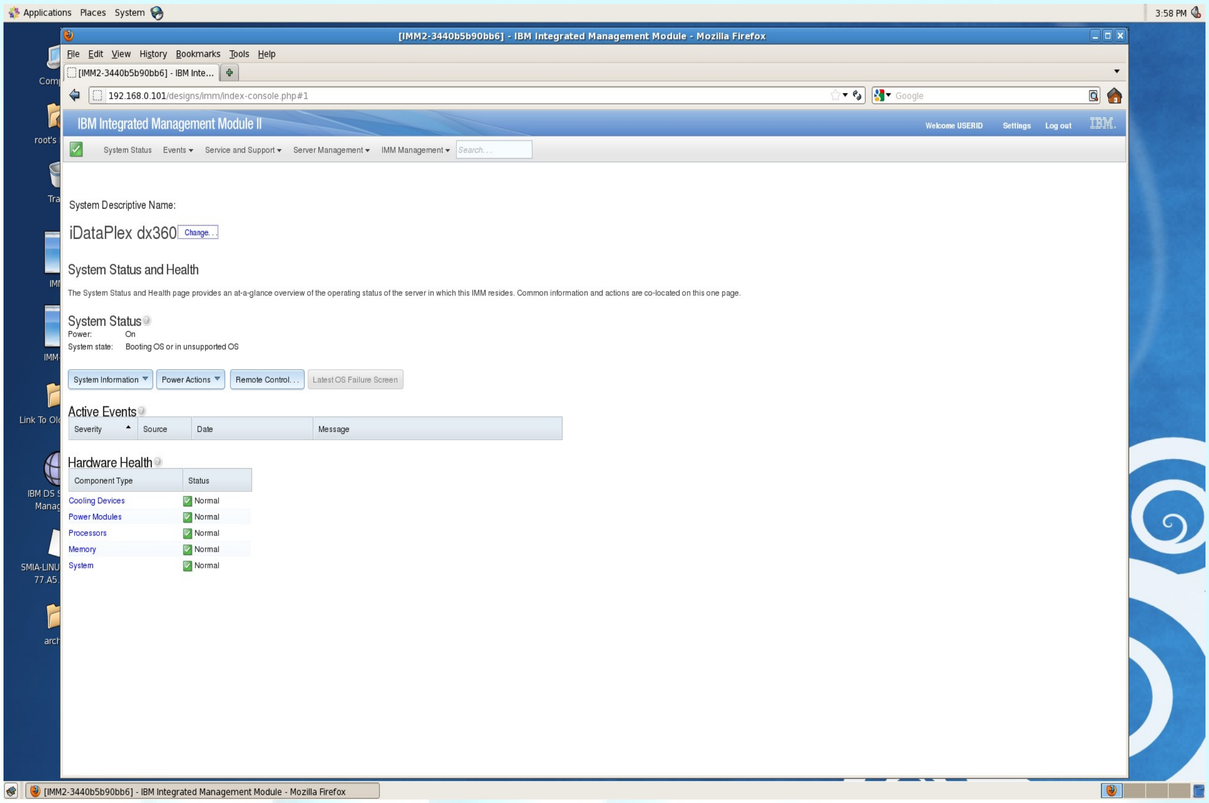
Supported Browsers

Licensed Materials - Property of IBM Corp. © IBM Corporation and other(s) 2010. IBM is a registered trademark of the IBM Corporation in the United States, other countries, or both.

Figure 3.10: IMM Login Screen

3. On the Welcome Web page, select a timeout value from the drop-down list in the field that is provided. If our browser is inactive for that number of minutes, the IMM logs off the Web interface.

   Note: Depending on how our system administrator configured the global login settings, the timeout value might be a fixed value.
4. Click Continue to start the session. The browser opens the System Status page, which gives us a quick view of the server status and the server health summary.



Applications Places System
3:58 PM
[IMM2-3440b5b90bb6] - IBM Integrated Management Module - Mozilla Firefox
File Edit View History Bookmarks Tools Help
192.168.0.101/designs/imm/index-console.php#1
IBM Integrated Management Module II
Welcome USERID Settings Log out
System Status Events Service and Support Server Management IMM Management Search...

System Descriptive Name:

iDataPlex dx360 Change...

System Status and Health

The System Status and Health page provides an at-a-glance overview of the operating status of the server in which this IMM resides. Common information and actions are co-located on this one page.

System Status

Power: On

System state: Booting OS or in unsupported OS

System Information
Power Actions
Remote Control...
Latest OS Failure Screen

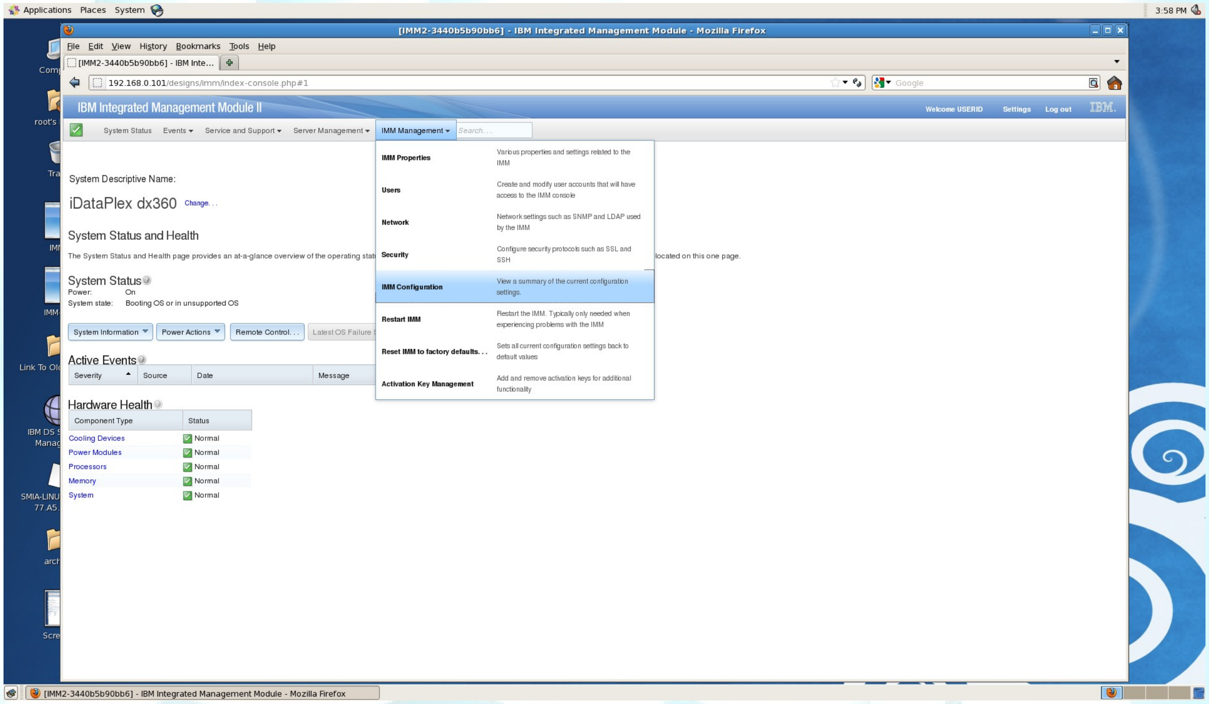
Active Events

Severity	Source	Date	Message

Hardware Health

Component Type	Status
Cooling Devices	✓ Normal
Power Modules	✓ Normal
Processors	✓ Normal
Memory	✓ Normal
System	✓ Normal

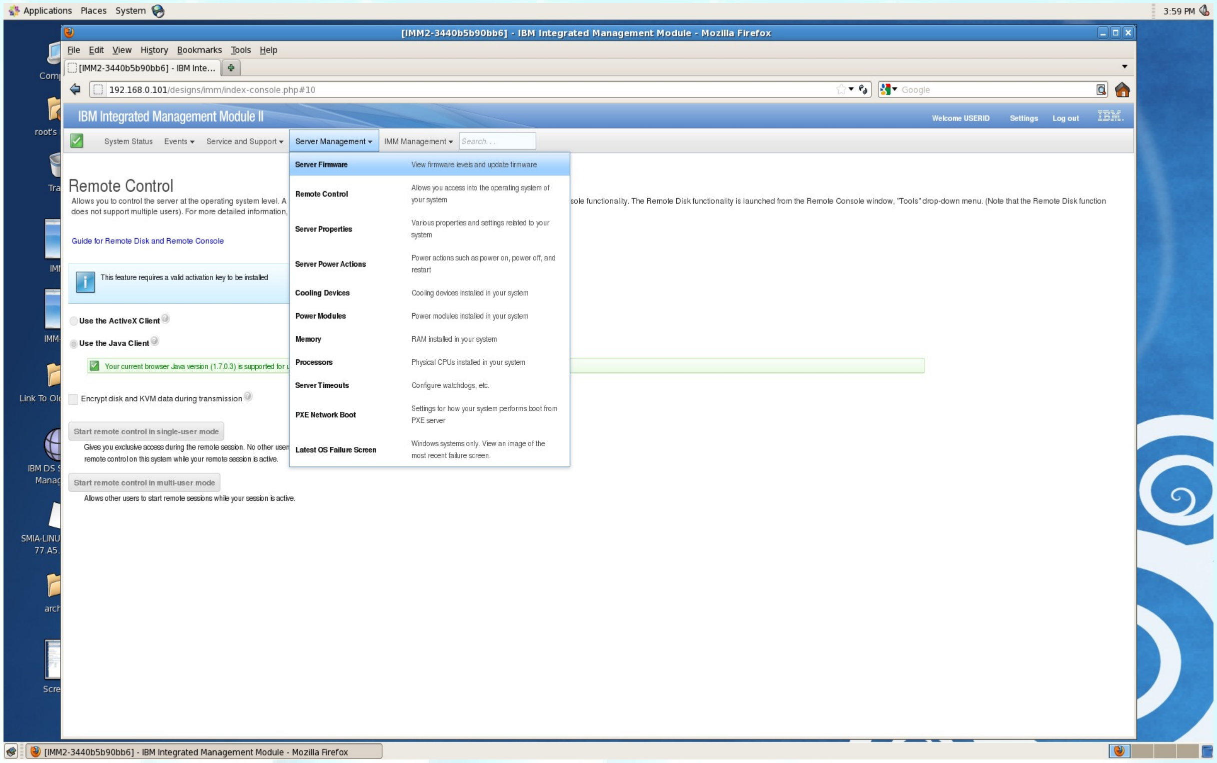
Figure 3.11: System Status Page of IMM



Applications Places System
3:58 PM
[IMM2-3440b5b90bb6] - IBM Integrated Management Module - Mozilla Firefox
IBM Integrated Management Module II
IMM Management

IMM Properties	Various properties and settings related to the IMM
Users	Create and modify user accounts that will have access to the IMM console
Network	Network settings such as SNMP and LDAP used by the IMM
Security	Configure security protocols such as SSL and SSH
IMM Configuration	View a summary of the current configuration settings.
Restart IMM	Restart the IMM. Typically only needed when experiencing problems with the IMM
Reset IMM to factory defaults...	Sets all current configuration settings back to default values
Activation Key Management	Add and remove activation keys for additional functionality

Figure 3.12: IMM Management.


Applications Places System
3:59 PM
[IMM2-3440b5b90bb6] - IBM Integrated Management Module - Mozilla Firefox
File Edit View History Bookmarks Tools Help
[IMM2-3440b5b90bb6] - IBM Inte...
192.168.0.101/designs/imm/index-console.php#10
Google
IBM Integrated Management Module II
Welcome USERID
Settings
Log out
IBM.
System Status
Events
Service and Support
Server Management
IMM Management
Search...
Comp
root's
Tra
IMI
IMM-
Link To Ol
IBM DS S
Manag
SMIA-LINU
77.A5.
arch
Scre
[IMM2-3440b5b90bb6] - IBM Integrated Management Module - Mozilla Firefox

Remote Control

Allows you to control the server at the operating system level. A ... sole functionality. The Remote Disk functionality is launched from the Remote Console window, "Tools" drop-down menu. (Note that the Remote Disk function does not support multiple users). For more detailed information,

Guide for Remote Disk and Remote Console

This feature requires a valid activation key to be installed

○ Use the ActiveX Client

○ Use the Java Client

☑ Your current browser Java version (1.7.0.3) is supported for u

□ Encrypt disk and KVM data during transmission

Start remote control in single-user mode

Gives you exclusive access during the remote session. No other user ... remote control on this system while your remote session is active.

Start remote control in multi-user mode

Allows other users to start remote sessions while your session is active.

Server Firmware	View firmware levels and update firmware
Remote Control	Allows you access into the operating system of your system
Server Properties	Various properties and settings related to your system
Server Power Actions	Power actions such as power on, power off, and restart
Cooling Devices	Cooling devices installed in your system
Power Modules	Power modules installed in your system
Memory	RAM installed in your system
Processors	Physical CPUs installed in your system
Server Timeouts	Configure watchdogs, etc.
PXE Network Boot	Settings for how your system performs boot from PXE server
Latest OS Failure Screen	Windows systems only. View an image of the most recent failure screen.

Figure 3.14: IMM Server management.

5. Startup and Shutdown Procedures

Startup Sequence

Step1. Power on the IBM System Storage DS3510. After few minutes check all the led showing the green light.

Step2. Power on the IBM x3650 M4 server using the power button located at the front of the server. Check with the console that it has booted normally.

Step3. Check whether the storage has been mounted on the master server using df –h command.

```
root@Kohinoor ~] df –h
```

Step4. Power on all the compute nodes as well has GPU nodes using the power button in the front.

Step5. Check all the file systems are mounted properly. If not run the command

```
Rocks run host “hostname; mount –a”
```

```
root@Kohinoor ~] rocks run host “hostname; mount –a”
```

ShutDown Sequence

Step1. Unmount the storage mounted on all the server using the command

Compute nodes

```
root@Kohinoor ~] rocks run host “hostname; umount /scratch”

root@Kohinoor ~] rocks run host “hostname; umount /scratch2”

root@Kohinoor ~] rocks run host “hostname; umount
/export/home”
```

Master node

```
root@Kohinoor ~] Umount /scratch

root@Kohinoor ~] Umount /scratch

root@Kohinoor ~] Umount /export/home
```

Step2. Shut down the compute and gpu nodes

```
root@Kohinoor ~] Rocks run host “hostname; init 0”
```

Step3. Shut down the master node

```
root@kohinoor ~] Init 0
```

6. scalation Matrix

Service Desk Timings: 09:15 Hrs to 18:00 (Monday to Friday)		
HPC Support		
Response Time	4 Hrs.	
Level 1	Mr. Nitesh	
	Helpdesk	
	040-30509117	
	support@locuz.com	
Level 2		
	Mr. Narender gaddam	Mr. Sangamesh
	Sr. System Engineer	Sr.Consultant-HPC
	040-30509230	080-40506868-6820
	91-	91-9986746471
	Narender.gaddam@locuz.com	Sangamesh.banappa@locuz.com
Level 3		
	Mr. Srinivas	
	Service Delivery Manager	
	040-30509117	
	91-9885035972	
	Srinivas.i@locuz.com	
Level 4		
	Srinivas Chada	
	GM-Availability Services & Operations	
	040-30509277	
	91-9949545672	
	sreenivas.chada@locuz.com	