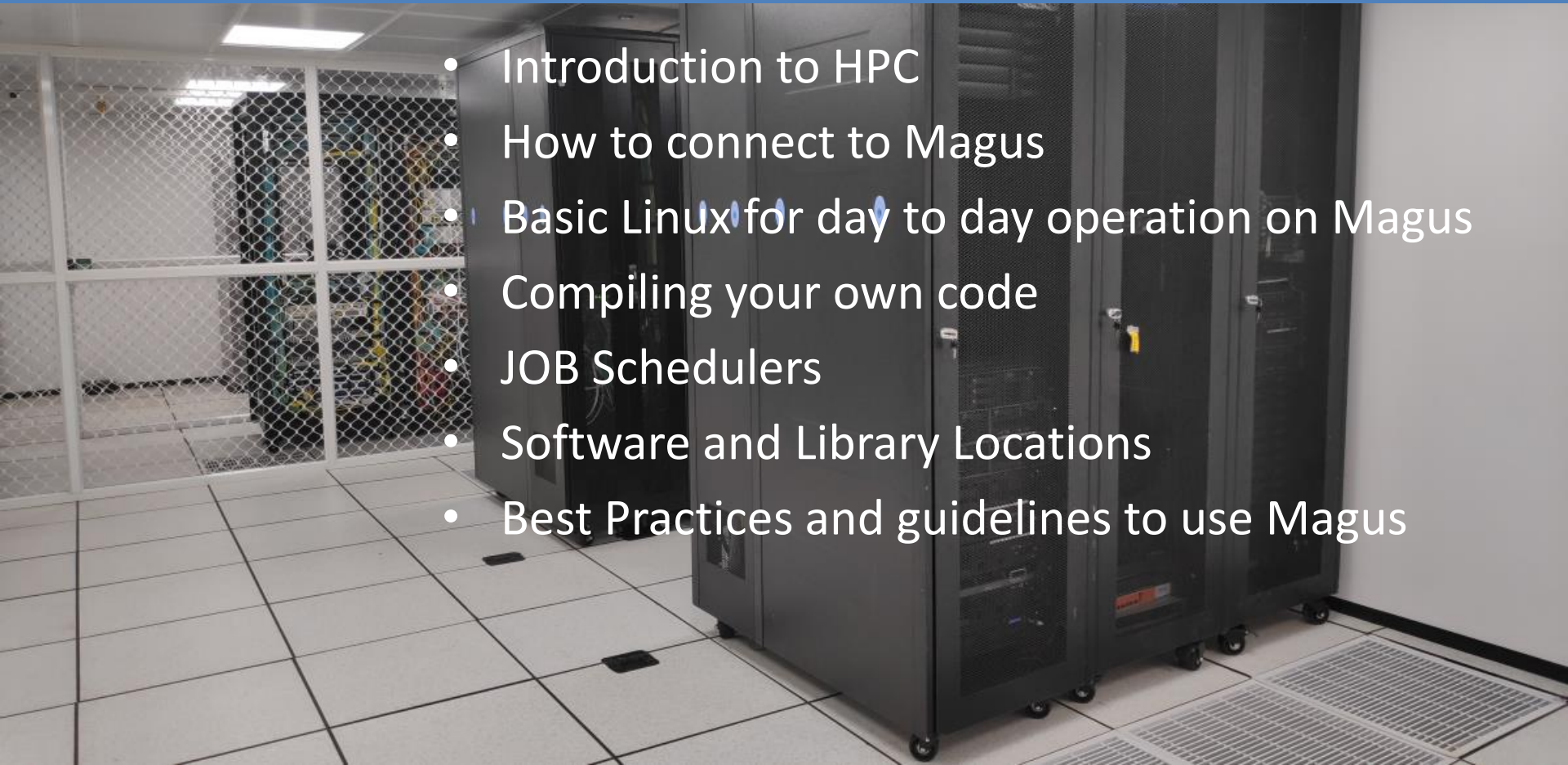




HPCC- MAGUS- Introduction.

Objectives

- Introduction to HPC
- How to connect to Magus
- Basic Linux for day to day operation on Magus
- Compiling your own code
- JOB Schedulers
- Software and Library Locations
- Best Practices and guidelines to use Magus



- What is HPC and why is it different to using your desktop?

“High Performance Computing most generally refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business.” -insideHPC

- Aggregated computing power
- Very large problem sizes
- Multiple problems simultaneously
- Large Data sets

Parallel Computing

- **Example of Serial Computing.**

- $(5+2) + (3*4) * 2*(100-(2+4))$

- $7+(3*4)*2*(100-(2+4))$

- $7+12*2*(100-(2+4))$

- $7+12*2*(100-6)$

- $7+12*2*94$

- $7+24*94$

- $7+2256$

- Result 2263

- Total Cycles Used 7

- **Using Parallel Computing**

- **Using 3 nodes**

	Node 1	Node 2	Node 3
Cycle 1	(5+2)	(3*4)	(2+4)
Cycle 2	100-6	12*2	Idle
Cycle 3	24*94	idle	Idle
Cycle 4	7+2256	idle	idle

Result : 2263

Total Cycle used 4

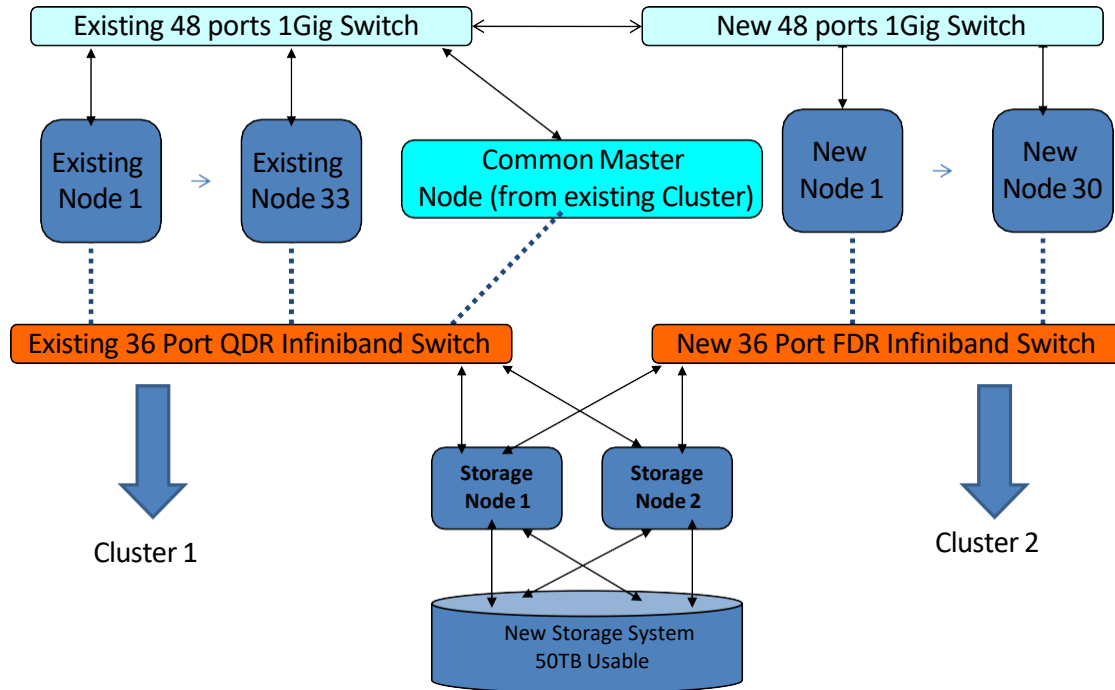
SNU HPCC- Magus – Key facts

- **Total 62 Compute Nodes.**
- **New Intel Hash well Architecture Processors on 30 Nodes**
- **Total ~ 1000 Cores**
- **Total ~ 6 TB RAM.**
- **IBM GPFS Parallel File System**
- **~30 TF Theoretical Peak Performance Total.**
- **8- High CPU & Memory Nodes**
- **Cluster Management Software :-
IBM Platform HPC**



SNU HPC- Magus Architecture

HPC Cluster Layout for SNU



Request for User Account on HPC.
<http://hpc.snu.edu.in/hpcAccount>

 HPC User Account Request Form

User Type

User Name

Email ID

Department

School

Research Group

Abstract of Research Project

Softwares you want to use

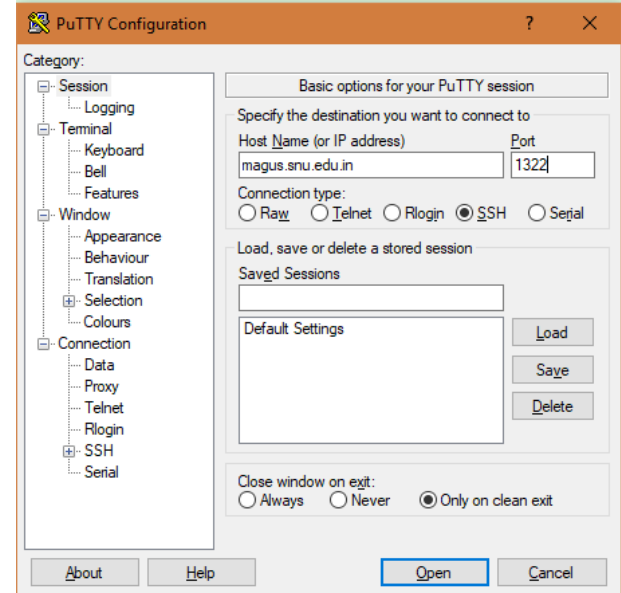
Account Expiry

Other Comments

I Agree to comply acceptable Use Policy

How to Connect to Magus

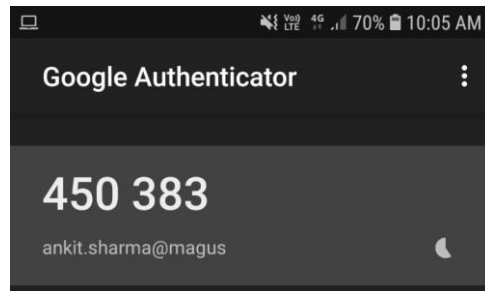
- **SSH**
 - Host `magus.snu.edu.in` (default port 1322)
- **From Linux Machine**
 - `$ ssh user@magus.snu.edu.in -p 1322`
- **From Windows Machine using putty**



Connect to Magus from outside SNU Network

9

- **Similar process as you connect within SNU network**
- **Additional Layer of security with Google Authenticator**
- **User needs to enter the verification code generated by the Google Authenticator App**
- **Once successful. Then the user needs to enter the password to login**



```
magus.snu.edu.in - PuTTY
login as: ankit.sharma
Using keyboard-interactive authentication.
Verification code: █
```

```
magus.snu.edu.in - PuTTY
login as: ankit.sharma
Using keyboard-interactive authentication.
Verification code:
Using keyboard-interactive authentication.
Password: █
```

Reference Url: http://wiki.snu.edu.in/index.php/Google_Authenticator

How to move data In/Out from HPC

SCP General Syntax

```
scp source_file_name username@destination_host:destination_folder
```

SCP commonly used flags

- P port : Specifies the port to connect to on the remote host.
- p : Preserves modification times, access times, and modes from the original file.
- q : Quiet mode: disables the progress meter as well as warning
- r : Recursively copy entire directories.
- C : Compress Data while copy.
- v : Verbose mode.

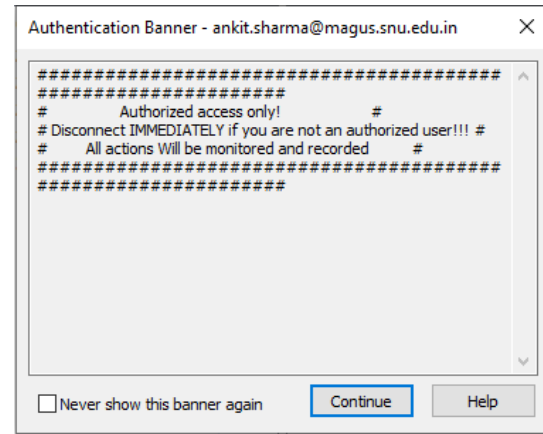
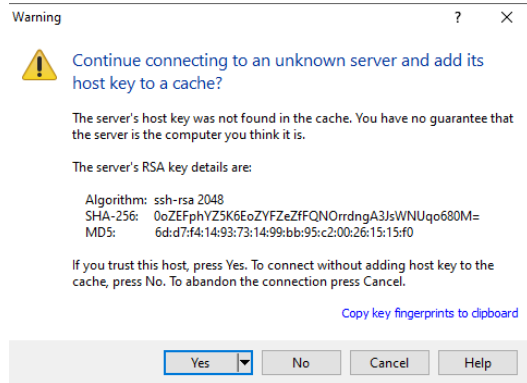
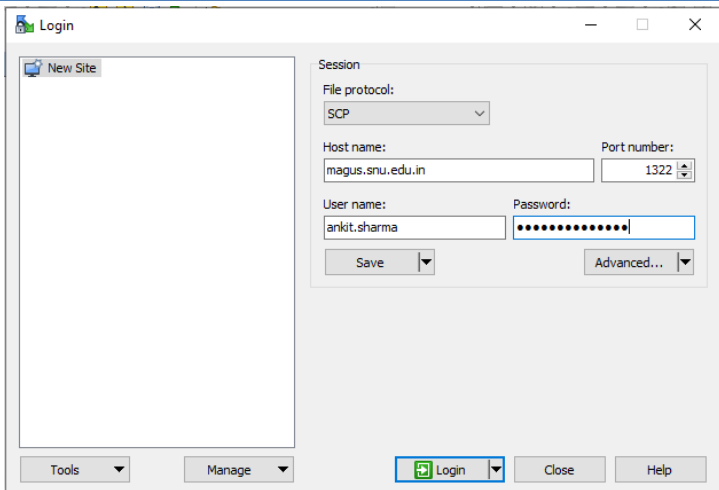
Sample file transfer

```
[root@backup ~]# scp -rC -P 1322 ankit.txt ankit.sharma@magus.snu.edu.in:/snufs/home/ankit.sharma/
#####
#           Authorized access only!           #
# Disconnect IMMEDIATELY if you are not an authorized user!!! #
#           All actions Will be monitored and recorded           #
#####
Verification code:
Password:
Copyright (c) 2009-2014 Intel Corporation. All rights reserved.
[root@backup ~]# █
```



Best Practise: Data Transfer Location must be your Home Dir: /snufs/home/<user.name>/

Data Transfers using WinSCP Windows (Client)



C:\Users\AnkitSharma\Documents\				/snufs/home/ankit.sharma/				
Name	Size	Type	Changed	Name	Size	Changed	Rights	Owner
↑		Parent directory	24-10-2019 10:07:29 AM	↑		01-10-2019 04:24:40 PM	rw-r--r--	root
Custom Office Templ...		File folder	24-10-2019 10:07:29 AM	amber18		16-10-2019 05:21:05 PM	rw-rw-r--	ankit.s...
SQL Server Managem...		File folder	22-10-2019 11:37:30 AM	Apps		25-09-2019 04:06:05 PM	rw-rw-r--	ankit.s...
Virtual Machines		File folder	22-10-2019 02:10:43 PM	downloads		16-10-2019 02:34:22 PM	rw-rw-r--	ankit.s...
Visual Studio 2010		File folder	30-09-2019 03:21:24 PM	intel		23-09-2019 02:57:21 PM	rw-r--r--	ankit.s...
				others		23-09-2019 02:28:30 PM	rw-rw-r--	ankit.s...
				workingdir		23-09-2019 02:51:45 PM	rw-rw-r--	ankit.s...
				1	1 KB	24-10-2019 10:42:28 AM	rw-rw-r--	ankit.s...

Magus Login Screen

```
login as: deepak
Pre-authentication banner message from server:
| #####
| # Authorized access only! #
| # Disconnect IMMEDIATELY if you are not an authorized user!!! #
| # All actions will be monitored and recorded #
| #####
End of banner message from server
Keyboard-interactive authentication prompts from server:
Password:
End of keyboard-interactive prompts from server
Last login: Thu Oct 24 09:51:14 2019 from 10.5.6.183
IBM Platform HPC 4.2 (build 243748) Management Node

=====
Welcome to magus.snu.edu.in HPC @ Shiv Nadar University(http://snu.edu.in)

Warning: Access Allowed to Authorized Users only.
***** Disconnect IMMEDIATELY if you are not authorized *****
=====

          MAGUS

#####
+++++ Host System Data :+++++
- Hostname = magus.snu.edu.in
- Address = 180.179.193.116
- Kernel = 2.6.32-431.el6.x86_64
- Uptime = 09:57:44 up 206 days, 11:28, 6 users, load average: 5.17, 4.14, 3.80
+++++ Cluster Data :+++++
----- Computing Nodes ----- #RAM/n --- #Cores ---
+compute-[01-22] (2 Xeon E5-2640v3@2.60Ghz [8c ] ) 64GB 352
+compute-[23-30] (2 Xeon E5-2670@2.60Ghz [8c ] ) 256GB 128
+compute-[31-60] (2 Xeon E5-2670@2.60Ghz [8c ] ) 64GB 480
+gpu-[01-02] (2 Xeon E5-2670@2.60Ghz [8c ] ) 64GB 32
+ 2x4 GPU accelerator (Tesla [K10]) +12288
=====
*** TOTAL: 62 nodes, 992 cores (+ 12288 GPU cores) ***
-----
+ Interconnect = InfiniBand QDR 40 Gb/s and FDR 56Gb/s
+ Shared Storage = 50 TB GPFS, Free: 7.0T Used(87%)
+++++ User Data :+++++
- Username = deepak
- Pending Jobs = 0
+ Running Jobs = 0
+++++ Support & Maintenance Information :+++++
- Wiki.....http://wiki.snu.edu.in/index.php/HPC
- FAQ.....http://wiki.snu.edu.in/index.php/HPC\_FAQ
- HPC Admin.....hpc\_admin@snu.edu.in |
- Support Email.....ithelpdesk@snu.edu.in |
- Phone: .....(+91)0120 7170105 |
+++++
*****Magus is currently under Production.*****
Warning: Do not submit jobs on master node. Such
jobs will be killed and userid will be reported.
+++++
```

Basic Linux CLI Commands

- **man (Manual)**
- **ls (list directory)**
- **mkdir (Make Directory)**
- **rmdir (Remove Directory)**
- **pwd (present working Directory)**
- **cp (Copy)**
- **mv (Move / Rename)**
- **scp (Secure copy to other machine)**
- **cat (Display contents of the file)**
- **tail (Display last 10 lines)**
- **head (display first 10 lines)**
- **chmod (Change File permissions)**
- **grep (Search within files)**
- **du (Disk Usage)**
- **wc (word count)**

Shortcuts

- **Ctrl+C (kill a running command)**
- **Ctrl+Z (suspend a running command)**
- **fg/bg (Foreground and Background)**
- **Ctrl+R (search recent commands)**

- **Standard Output Redirection using > and >>**
- **Standard Error Redirection 2 >**
- **Sending command to background using &**
- **Sending output to other command using Pipe |**

Compiling your code

- **Compiling a simple Hello World in C on linux**
- **Compiling a MPI Hello World in C on linux**
- **How to set environment variables for location of compilers and mkl libraries.**
 - ○ *\$ source /snufs/intel/parallel_studio_xe_2015/bin/psxevars.sh intel64*

Sample Mpi Hello World

```
#include<stdio.h>
```

```
#include<mpi.h>
```

```
int main(int argc, char *argv[])
```

```
{
```

```
    int ranks, rank, n;
```

```
    int Debugmode=1;
```

```
    MPI_Init(&argc, &argv);
```

```
        char node[MPI_MAX_PROCESSOR_NAME];
```

```
        MPI_Comm_size(MPI_COMM_WORLD, &ranks);
```

```
        MPI_Comm_rank(MPI_COMM_WORLD, &rank);
```

```
        MPI_Get_processor_name(node,&n);
```

```
        printf("Greetings: %d of %d from the node %s\n", rank, ranks, node);
```

```
    MPI_Finalize();
```

```
    return 0;
```

```
}
```


- **Setting environment variables**

```
$ source /snufs/intel/parallel_studio_xe_2015/bin/psxevars.sh intel64
```

- **Compiling**

```
$ mpiicc
```

- **Executing mpi jobs**

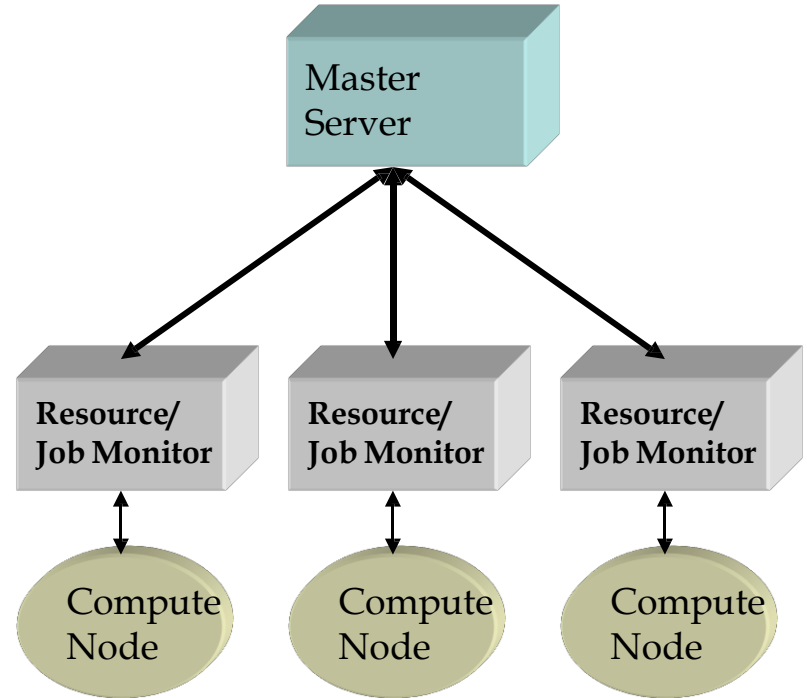
```
$ mpirun -np <number of processors> -f <hostfile>
```

- **Mpirun options.**

- ppn Processor per node

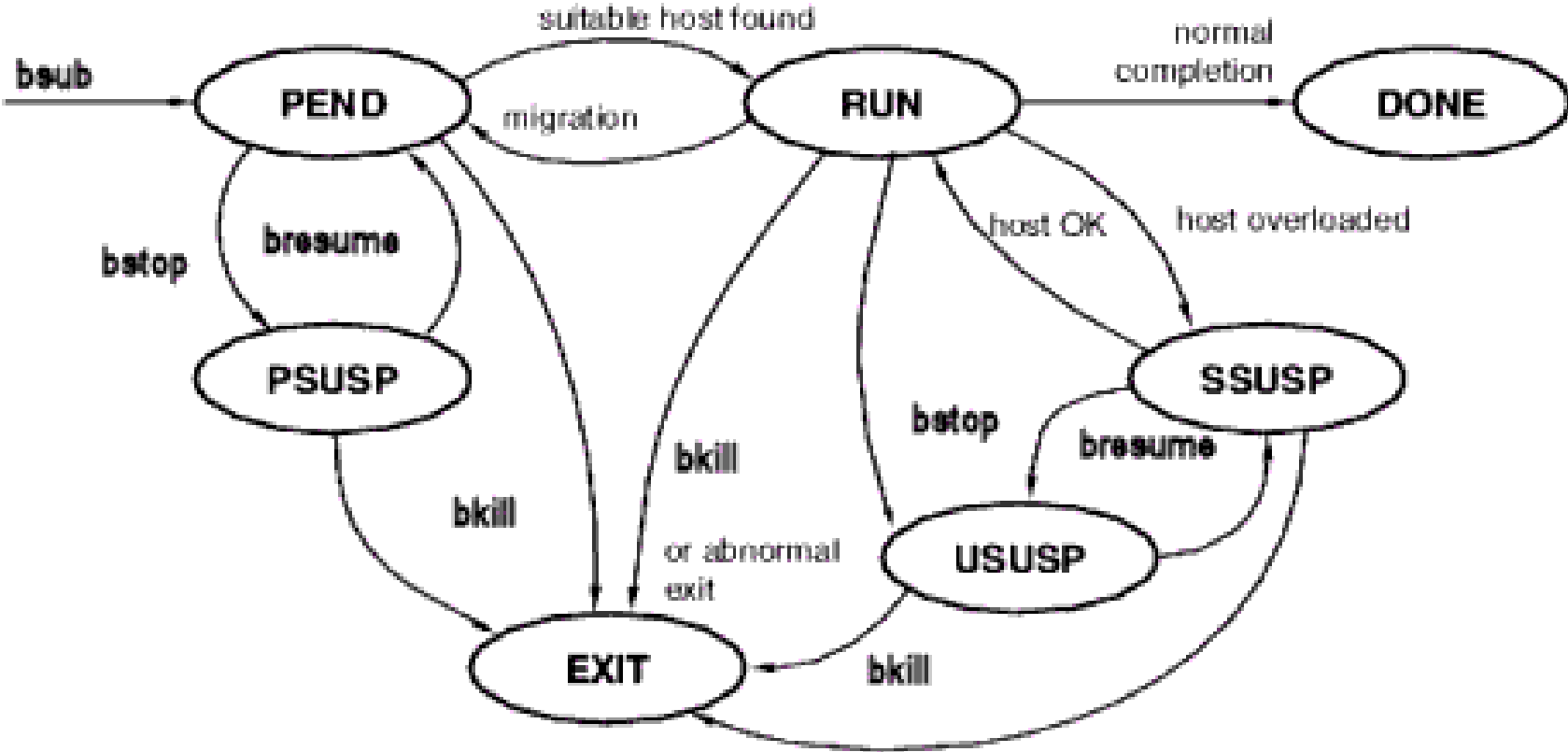
Job Scheduler

- Allow users to share computing resources
- Utilize resources efficiently.
- **IBM Platform LSF**
 - distributed workload management solution for maximizing the performance of High Performance Computing (HPC) clusters.



- **LSF jobs have the following states:**
 - **PEND** — Waiting in a queue for scheduling and dispatch
 - **RUN** — Dispatched to a host and running
 - **DONE** — Finished normally with zero exit value
 - **EXIT** — Finished with non-zero exit value
 - **PSUSP** — Suspended while pending
 - **USUSP** — Suspended by user
 - **SSUSP** — Suspended by the LSF system

Job Transitions



- **A cluster wide container for jobs. All jobs wait in queues until they are scheduled and dispatched to hosts.**
- **Queues do not correspond to individual hosts; each queue can use all server hosts in the cluster, or a configured subset of the server hosts.**
- **When you submit a job to a queue, you do not need to specify an execution host. LSF dispatches the job to the best available execution host in the cluster to run that job.**
- **Queues implement different job scheduling and control policies.**

Queues on Magus

S.No.	Processor Architecture	Priority	Queue Name	Min no of cores required to submit job	Max no of cores allowed per job	No of nodes in the queue	Wall Time	Max job per users in the Queue based on max cores
1	SandyBridge	50	serial_short	1	1	1	1 hour	unlimited
2	SandyBridge	50	serial_long	1	1	1	1 month	4
3	SandyBridge	50	short_sdb	4	8	12	3 days	32
4	SandyBridge	50	med_sdb	8	32	12	2 weeks	32
5	Hashwell	50	high_mem	16	32	8	1 month	32
6	SandyBridge	50	large_sdb	16	16	4	1 month	16
7	Hashwell	50	large_hsw	16	16	4	1 month	16
8	Hashwell	50	med_hsw	8	32	18	2 weeks	32
9	SandyBridge	50	GPU	16	16	2	1 week	16
10	SandyBridge	20	long_gpu	16	32	2	1 week	16
11	SandyBridge	20	long_sdb	8	32	20	1 month	unlimited
12	Hashwell	20	long_high_mem	8	32	8	1 month	unlimited
13	Hashwell	20	long_hsw	8	32	20	1 month	unlimited

Job Submission

```
$ bsub < jobfile
```

```
#!/bin/bash
#BSUB -J Helloworld
#BSUB -n 16
#BSUB -q high_mem
#BSUB -e error.%J
#BSUB -o out.%J
#BSUB -u "deepak.agrawal@snu.edu.in"
#BSUB -N
#BSUB -W 10:00
#BSUB -m compute26
```

bsub options

-B	Sends email when the job is dispatched
-H	Holds the job in the PSUSP state at submission
-I	Submits a batch interactive job.
-K	Submits a job and waits for the job to finish
-N	Emails the job report when the job finishes
-x	Exclusive execution on host
-b	begin_time Dispatches the job on or after the specified date and time in the form [[month:]day:]:minute
-e	error_file Appends the standard error output to a file
-E	"pre_exec_command[arguments...]" Runs the specified pre-exec command on the execution host before running the job
-J	"job_name" Assigns the specified name to the job.
-q	queuename Submits jobs to the specified queue
-o	output_file Appends to standard output to a file
-u	email address < sets the email where the email has to be sent >

LSF Sample Submission script

```
#!/bin/bash
#BSUB -J Hello world
#BSUB -n 16
#BSUB -q high_mem
#BSUB -e error.%J
#BSUB -o out.%J
#BSUB -R "span[ptile=16]"
```

```
MPI=16 PPN=16
MYDIR=$(pwd)
```

```
EXE=/snufs/home/deepak/helloworld/a.out
OUT_FILE=$MYDIR/out.log
```

```
# Do not change anything below this
export I_MPI_DAPL_PROVIDER=ofa-v2-mlx4_0-1
export I_MPI_FABRICS=shm:dapl
export I_MPI_FALLBACK=0
export OMP_NUM_THREADS=1
export FORT_BUFFERED=yes
export I_MPI_PIN_PROCESSOR_LIST=0-15
rm -f host.list
cat $LSB_DJOB_HOSTFILE > ./host.list env > log.env
mpiexec.hydra -np $MPI -f ./host.list -genvall -ppn $PPN $EXE 2>&1 | tee -a $OUT_FILE
```

- **Kill a running Job**
 - `$ bkill < jobid>`
- **See the status of your jobs in the Queue**
 - `$ bjobs`
- **See status of all user jobs**
 - `$ bjobs -u all`
- **See Information about Queues**
 - `$ bqueues`
- **See Resources on hosts**
 - `$ bhosts`

- **Environment Variables in .bashrc**
 - `source /snufs/intel/composer_xe_2015.2.164/bin/compilervars.sh intel64`
 - `source /snufs/intel/impi/5.0.3.048/intel64/bin/mpivars.sh`
- **Location of VASP-5.3.5 Binaries.**
 - **Vasp for Hashwell**
 - `/snufs/apps/vasp/5.3.5/intelmpi/vasp.hw`
 - `/snufs/apps/vasp/5.3.5/intelmpi/vasp.hw.gamma`
 - `/snufs/apps/vasp/5.3.5/intelmpi/vasp.hw.nc`
 - **Vasp binaries for Sandybridge**
 - `/snufs/apps/vasp/5.3.5/intelmpi/vasp.sdb`
 - `/snufs/apps/vasp/5.3.5/intelmpi/vasp.sdb.gamma`
 - `/snufs/apps/vasp/5.3.5/intelmpi/vasp.sdb.nc`
- **Sample Job Script :** `/snufs/apps/vasp/5.3.5/intelmpi/submit.lsf.example`

- **Gromacs**
- **Vasp**
- **Quantum espresso**
- **BigDFT**
- **Lammps**
- **Gaussian**
- **USPEX**
- **Matlab (single node)**

Thank You

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