



High Performance Computing Cluster

Agenda

Basic Introduction

How to access Magus02

Understanding of Queues

Using Modules/Libraries

Working with Job Scheduler(Slurm)

Introduction to LiCO

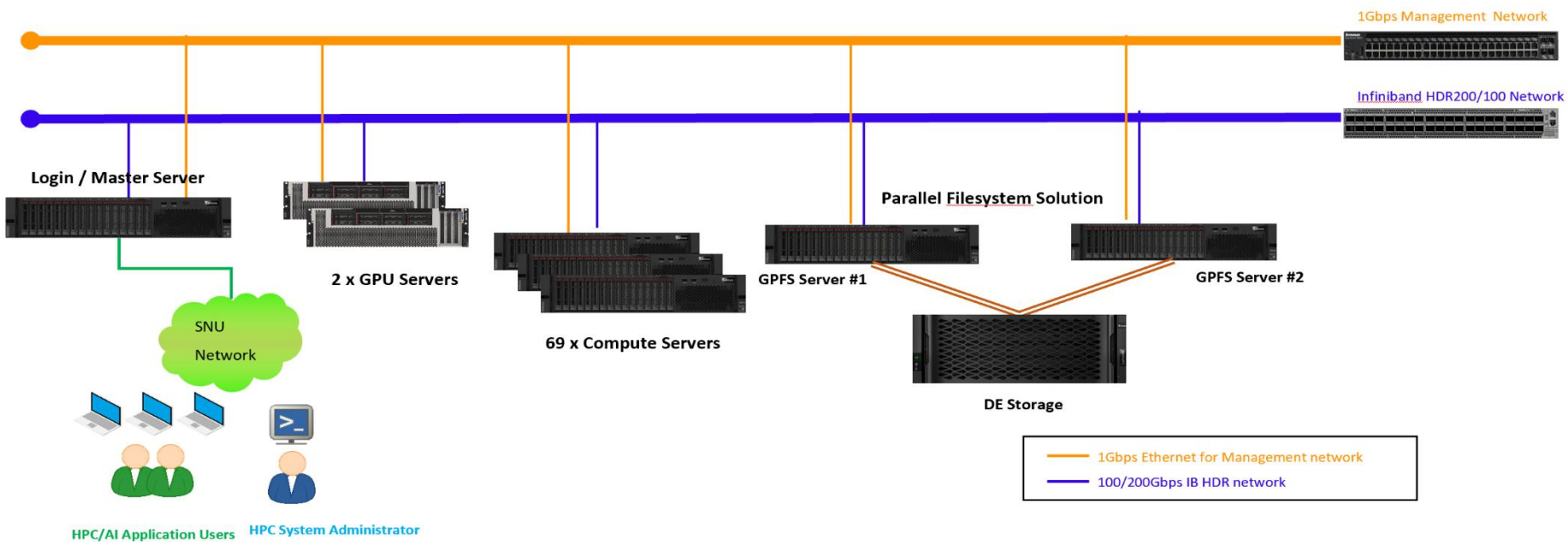
Question/Answer

Specification

- Total Cores = 8064 (AMD)
- 238 Tflops
- 57 Compute Nodes
- 2 Login Nodes
- 2 Master Nodes
- 12 High memory nodes with local **SSD**
 - Better performance of applications, which require high performance storage but do not scale well across nodes. E.g. Gaussian.
- Memory
 - 4GB Per core for Compute Nodes, with a total memory = 29,184 GB
 - 16GB Per core for High Memory Nodes, with total memory = 12,288 GB

Compute Specification

COMPUTE NODES	PROCESSOR	RAM	CORE	GPU	NO OF NODES	TOTAL RAM	TOTAL CORES
Compute Node	AMD EPYC 7763	512 GB	128		57	29184 GB	7296
High Memory Node	AMD EPYC 7543	1024 GB	64		12	12228 GB	768
GPU	INTEL XEON PLATINUM 8358	512 GB	64	Tesla A100x4	2	1024 GB	128
Total					71	42436 GB	8192
Storage	750 TB PFS						



HPC/AI Application Users HPC System Administrator

System	Model	No.	Compute
IO Servers	SR665	2	SR645 - 57qty - AMD 7763 64C, 512G Mem SR645 - 12Qty - AMD 7543 32C, 1T Mem + <u>lscratch</u>
Login/Master Server	SR665	4	GPU
Compute nodes	SR645	57+12	SR670 -2 Qty – 8 * NVIDIA A100 80G GPU
Storage	DE6000H + DE600S	2	Storage 16TB – Scratch – SSD 520TB – Data-Home – SSD + HDD

Architecture Diagram

How to connect Magus02

The image shows two windows from a Linux desktop environment. On the left is the 'PuTTY Configuration' dialog box, and on the right is a terminal window.

PuTTY Configuration Dialog:

- Category:** SSH
- Basic options for your PuTTY session:**
 - Specify the destination you want to connect to:
 - Host Name (or IP address): magus02.snu.edu.in
 - Port: 22
 - Connection type: SSH Serial Other: Telnet
 - Load, save or delete a stored session:
 - Saved Sessions: (empty list)
 - Default Settings: (empty text box)
 - Buttons: Load, Save, Delete
 - Close window on exit: Always Never Only on clean exit
- Buttons: About, Open, Cancel

Terminal Window:

```
bhuvnesh@ln1:~  
login as: bhuvnesh  
bhuvnesh@magus02.snu.edu.in's password:  
Last login: Thu Feb 16 10:41:37 2023 from 10.5.32.56  
[bhuvnesh@ln1 ~]$
```

Queue Configuration

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 Cores User can Use in the Queue	Max No. of Pending Jobs Per user
1	AMD EPYC 7763	50	serial_test	1	8	1	1 hour	unlimited	unlimited
2	AMD EPYC 7763	50	medium	32	128	16	1 week	256	4
3	AMD EPYC 7543	50	small	8	32	16	1 weeks	128	1
4	AMD EPYC 7543	50	high_mem	32	256	10	2 weeks	256	1
5	AMD EPYC 7763	50	large	64	128	25	2 weeks	128	1
6	AMD EPYC 7543	50	large_io	8	32	2	1 weeks	32	1
7	Intel Xeon Platinum 8358	50	GPU	32	64	2	1 week	64	1

Modules / Libraries

module list

module av

module use

module
load/unload

Slurm (Job Script)

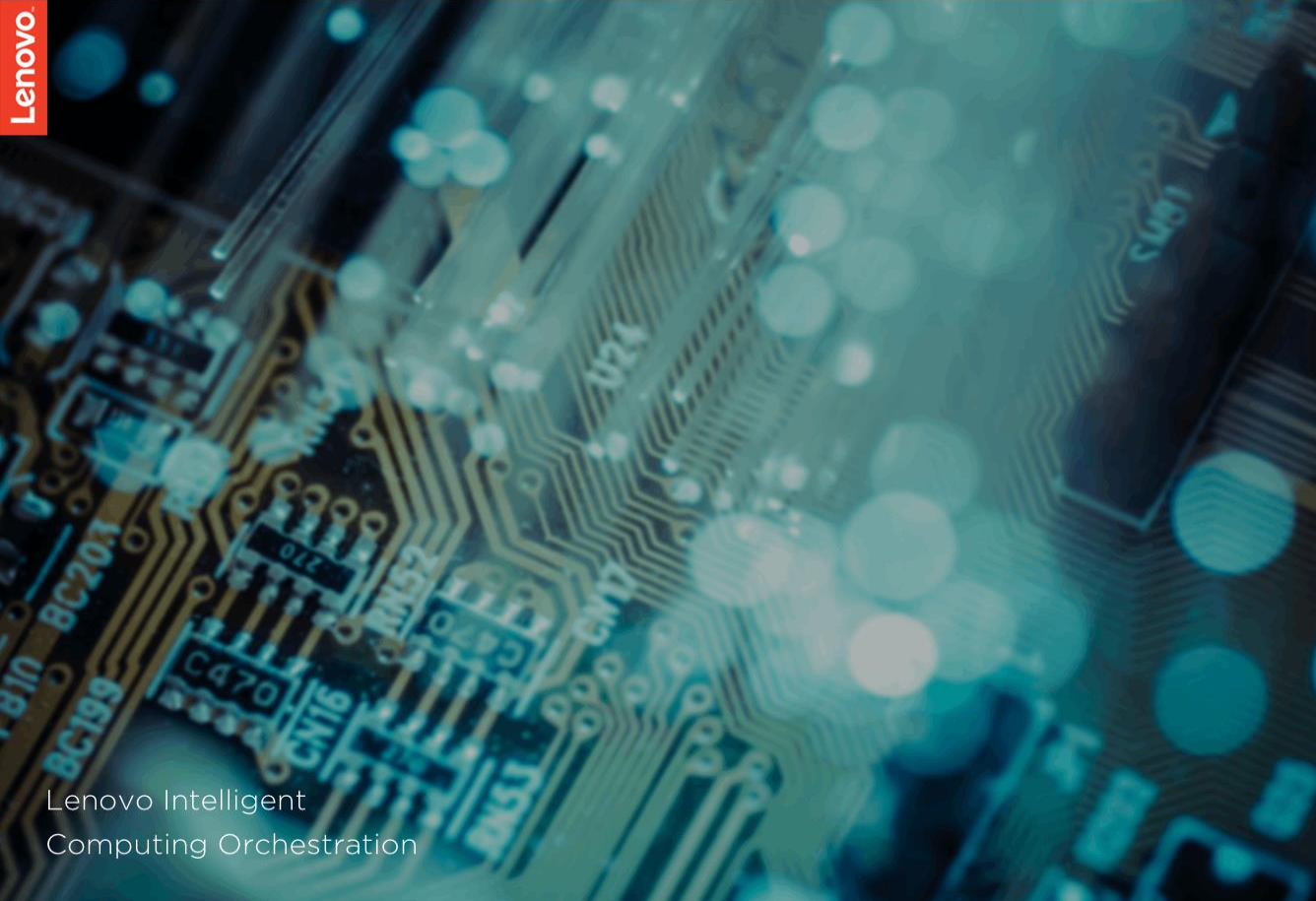
- `#!/bin/bash`
- `#SBATCH --partition=high_mem` # include the appropriate partition, node, ntasks, ntasks-pernode for the respective SLURM key
- `#SBATCH --nodes=1`
- `#SBATCH --ntasks=64`
- `#SBATCH --ntasks-per-node=64`
- `#SBATCH --cpus-per-task=1`
- `#SBATCH --exclusive`
- `#SBATCH --job-name=VASP`
- `#SBATCH --output vasp.%J.out`
- `#SBATCH --error vasp.%J.err`

- `###Inputs###`
- `### modify the appropriate version of the executable`
- `export exec_name=/data/apps/VASP/IntelMPI/5.4.4/bin/vasp_std`

Introduction to LiCO

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Lenovo



Lenovo Intelligent
Computing Orchestration



LiCO

Username

Please enter your Username.

Password

Log In

English ▾

Question/Answer