High Performance Computing at IPR

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Email: hpcteam@ipr.res.in
Computer Division, IPR

Presented By: Deepak Aggarwal

ANTYA

1 PETA FLOPs HPC System @ IPR

- Institute for Plasma Research, Gandhinagar has ANTYA - a 1 PETA FLOPs HPC system with more than 10000 cores.
- ANTYA is being extensively used by the academic, scientific, and engineering community of the Institute, by exploiting the power of parallel computing for solving their complex tasks.
- This system can perform 10^{15} **FL**oating-point **O**perations **P**er second. In Sanskrit, ANTYA implies 10^{15}!

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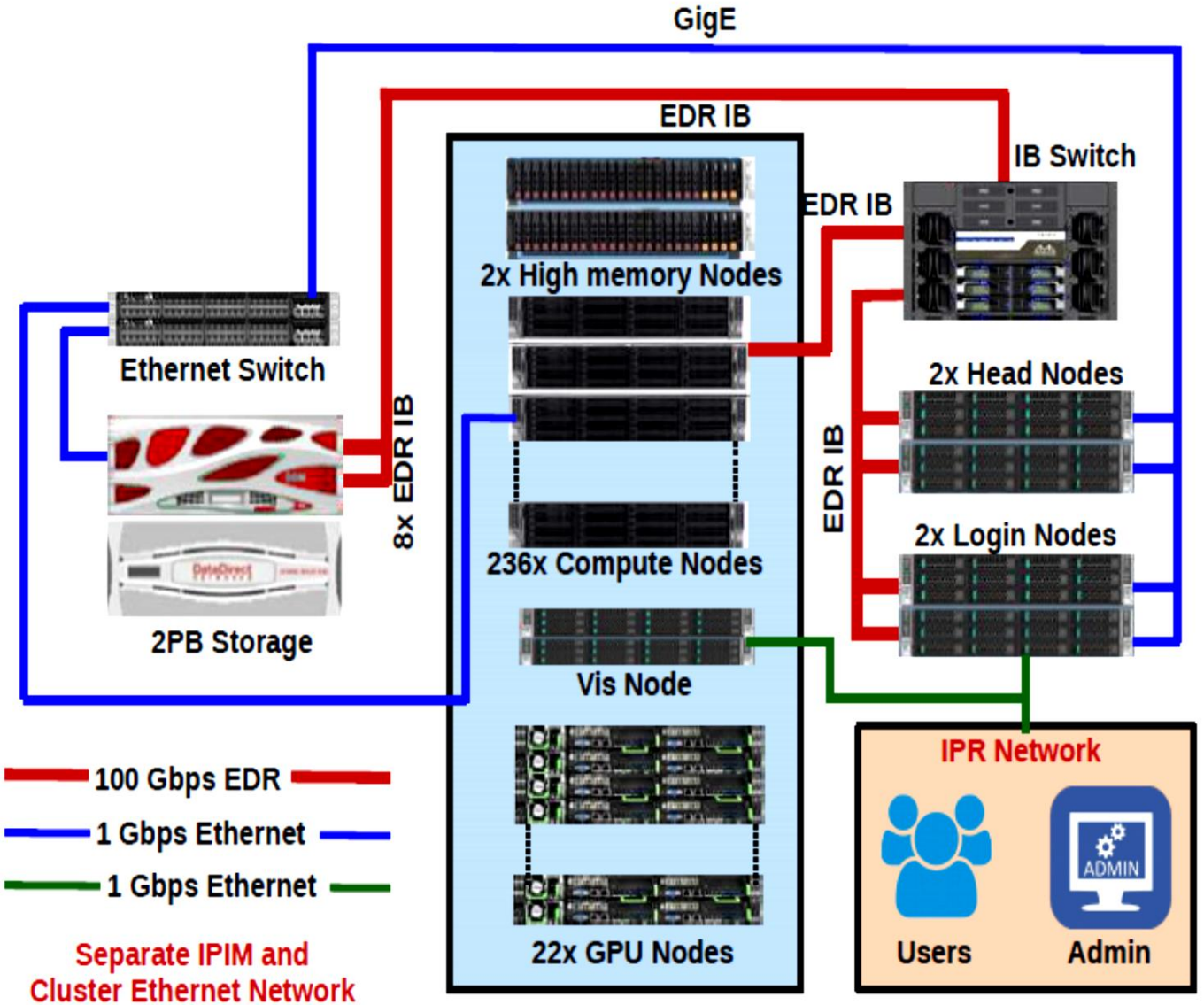
System Overview



System Includes

- Login Nodes – 02
- CPU Nodes – 236
  (40 Cores/Node)
- GPU Nodes – 22
  (2XP100 Cards/Node)
- Fat Nodes – 02
  (80 cores, 1TB RAM/Node)
- Viz. Node – 01
- Storage – 2 PetaByte (PB)

Performance

- Rpeak per node ~3.072 TF
- Cluster Rpeak ~ 1 PF
- Cluster Rmax ~ 620 TF

Software

- Red Hat (RHEL) – 7.5
- Scheduler – PBSPro

Login Nodes

- You should be connected to IPR network for accessing ANTYA.
- Login1 and Login2 are configured in round robin for balancing the load of the users.
- Please read the MOTD/flash screen just after the login for basic details about job submission.
- PBS Scheduler is used for job scheduling and monitoring
- Interactive as well as batch jobs can be submitted.

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Applications/Libraries/Compilers

- ANTYA has 53 libraries and more than 20 different codes installed - several of them indigenously developed or opensource as well as commercial licensed software which are being used for a variety of numerical simulations covering Computational Fluid Dynamics (CFD), Partile-In-Cell (PIC), Molecular Dynamics (MD), MHD, AI etc.

List of major codes being used in ANTYA

Open Source Codes	In-House Developed /Collaboration Codes*	Commercially Licensed Software for Engineering applications
LAMMPS • Multiscale modelling of radiation damage • Dusty plasma simulations. **PLUTO** • Recurrent and Non-Recurrent Flow Simulation • Astrophysical Dynamo simulation • MHD and strongly coupled plasma simulations • Studying plasma behaviour on accretion regimes. **OpenFOAM** • Deflagration to Detonation (DDT) Studies • Flooding simulations etc. **Bout++** • ITG instability simulations in a tokamak • Magnetic reconnection study in slab geometry • Edge and SOL region simulation in tokamak etc. **AI/ML/DL packages** Darknet yellow for real-time object detection, tensorflow and horowod usage for AI distributed training and development of intrusion detection software	**GMHD3D** (CPU and GPU versions, 3D) • Evolution of initial unstable magnetic and vorticity fields for Dynamo Problem, Self-consistent dynamo etc. • Study of Alfven wave in the 3D MHD plasma **EPPIC** (Expanding Plasma PIC, CPU and GPU version) • Study the physics of plasma in an expanding magnetic field **PEC2PIC** (2-D Parallelized Electrostatic Cartesian PIC) • Evolution of a pure electron plasma cloud in smartx **MPMD 2-D and 3-D** (Upgraded Multi-GPU version) • Large Scale MD Simulation **3D - MD Code** • Molecular Dynamics Simulations of Nano-Clusters **GTS*** **(**Gyrokinetic Tokamak Simulation) • Study of turbulence transport in tokamak **Osiris4.0*** (3-D, relativistic, object-oriented PIC code) • Laser plasma interaction simulations **Metis*** • Discharge scenario studies in a tokamak	**ANSYS** • Design of mechanical systems (ITER port, blanket module & pebble bed design • Thermo structural analysis of pyrolysis system • Heat transfer studies for plasma facing components (PFCs) • CFD study of twin-screw hydrogen extruder system, atmospheric plasma simulations etc. **COMSOL** • Magneto hydrodynamic Flow simulation in liquid breeder blankets • sheath & pre-sheath study in NI plasma etc. **CST** • Design of Passive Active Multijunction (PAM) launcher for ADITYA-U • Microwave/RF simulations for design of ICRH components • Meta-metarial studies etc.

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Applications/Libraries/Compilers

Serial Compilation for Single Core Codes

Language	GNU Compilers	Intel Compilers	PG Compilers
C	gcc	icc	pgcc
C++	g++	icpc	pgc++
Fortran	gfortran	ifort	pgfortran, pg77, pg90

Parallel Compilation for MPI Codes

Language	GNU Compilers (openmpi, mpich)	Intel Compilers
C	mpicc	mpicc/mpiicc
C++	mpicxx/mpic++/mpiCC	mpiicpc/mpicxx
Fortran	mpif77/mpif90/mpifort	mpif77/mpif90/mpiifort

Availing the Various Software Using the Environment Modules on ANTYA

- **Show the available software**

$ module avail

- **Show the available versions of a software**

$ module avail python

Show the available versions of a software

$ module load python385

- **Load the specific versions of a software from the available list**

$ module switch python385 python371

- **Switch to other version of a software**

$ module show python371

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Queuing Policy

Queue Name	Max Nodes (cores)	Max. Walltime	Max. Cores/job	Min. Cores/job	Max. R jobs/User	Max Q jobs/User	Max Q jobs/Queue	Relative Priority	Node Sharing	Node Binding	Remarks
debugq	3 (120)	30 min	No limit	No limit	2	1	5	Highest (First)	Yes	No	For the debugging of User-developed codes/applications.
regularq (~18%)	47 (1880)	96 hours	80	8	4	2	30	Second	No	No	Max. 160 cores or 4 running jobs per User at a time are allowed. Further, a User can submit 2 more jobs in the queue. 80 cores for jobs submitted on High Memory Nodes.
mediumq (60%)	156 (6240)	48 hours	1600	80	3	1	20	Third	No	No	Max. 1600 cores or 3 running jobs per User at a time are allowed. Further, a User can submit 1 more job in the queue.
longq (20%)	52 (2080)	120 hours	600	80	2	1	10	Lowest	No	No	Max. 600 cores or 2 running jobs per User at a time are allowed. Further, a User can submit 1 more job in the queue.
serialq (~2%)	5 (200)	15 days	10	1	20	4	20	Lowest	Yes	No	This queue is dedicated for serial code users.