सुस्वागत நல்வரவு ସୁସ୍ୱାଗତମ సుస్వాగతం સુસ્વાગતમ সুস্বাগতম ಸುಸ್ವಾಗತ സുസ്വാഗതം সুস্বাগতম ਸੁਆਗਤਮ सुस्वागतम् रंध्ش آمديد

23rd Aug 2021

### PARAM GANGA @ IIT Roorkee

 Ministry of Electronics and Information Technology
Government of India



# Agenda

PARAM-Ganga Architecture

Technical Specification of PARAM-Ganga

PARAM Ganga Software Stack

How to access Param-Ganga.

Ticketing Tool and Helpdesk

# PARAM GANGA

#### NSM HPC Users Service/Management Nodes (8 nos.) Firewall Secondary Communication ..... IPMI Login Nodes (8 nos.) Master Nodes (2 nos.) 10 G Compute Nodes (214 nos.) Storage L2 - Infiniband HDR **Primary Storage** 200 Gbps ------GPU Compute Nodes ------(20 nos.) -----L1 - Infiniband HDR 200 Gbps Archival Storage Compute -----Nodes with High memory (78 nos.) ----- Secondary (1G) 10G IPMI - Infiniband

#### **PARAM Ganga Architecture Diagram**



## **Technical Specifications**



#### **CPU only Compute Nodes**

- 214 Nodes
- 10272 Cores
- Compute power of Rpeak 953.156 TFLOPS
- Each Node with
  - 2\* Intel Xeon Platinum 8268, 24 cores, 2.9GHz, processors
  - 192 GB memory
  - 480 GB SSD

#### High Memory Compute Nodes

- 78 Nodes
- 3744 Cores
- Compute power of Rpeak 347.412 TFLOPS
- Each Node with
  - 2\* Intel Xeon Platinum 8268, 24 cores, 2.9GHz, processors
  - 768 GB memory
  - 480 GB SSD

#### **GPU Compute Nodes**

- 20 Nodes
- 800 CPU cores
- 204800 GPU Cores
- Compute power of Rpeak 64 TFLOPS + 280 TF = 344
- Each Node with
  - 2\* Intel Xeon Gold G-6248, 20 cores, 2.5 GHz, processors
  - 192 GB Memory
  - 480 GB SSD
  - 2xNvidia V100 SXM2 GPU cards each with 5120 CUDA cores

### **Software Stack**



	Performance Monitoring	HPCC		IMB	/osu			IOR	HPCG	
	Visualization Tools	Ferret		GrADS		ParaView		VisIt/ VMD	C-DAC Too IDE CAPO	
Programming Tools	Application Libraries	NetCDF/ H	IDF/ etc.	L	Math ibraries		l L	Python Ibraries	GNU Scientific Library	
	Development Tools	Intel Clus	ter Studio	D		GNU		CUDA 1	foolkit/ OpenACC	CHReM
	Communication Libraries	Intel N	ЛРІ	MI	/APICH2		O	oen MPI	PGAS	
	Cluster Monitoring/ Help Desk	Ganglia	C-D	AC Tools	5	Nag	ios	XDMoD	osTicket	C-Chaks SuPariksł
Middleware Applications	Resource Management/ Scheduling/ Accounting	SLURI		и			SLURM Acco		counting	SUM
and Management	Provisioning	OpenHPC (xCAT)						HPC Tas		
	File System	NFS		Loca	al FS (XFS	S)		Lustre	GPFS	Automat Scripts
Operating Systems	Drivers	OFED		CUD		Netv		work & Storage Drivers	Cluste	
	Operating System	Linux (CentOS 7.x)					Scripts			

# Software Components

### **Operating System –**

- HPC clusters generally are build with Linux operating system as a base OS (Centos7.6)
- It includes all the device drivers for the H/W connected to each node.

#### **Cluster Manager/Orchestrator**

- Tools in this category builds a centralized architecture where a controller node builds and manages the cluster.
- xCAT Is an open-source cluster Manager, Maintained by community, is the widely used tool for HPC as well as cloud clusters.
- It provides flexibility to handle objects within the cluster with its easy manageable methods
- It provide methods to deploy nodes with a very light weight stateless images.



#### **Resource Manager (SLURM)**

- As there are a lot of resource within a cluster like : CPU-Cores, Memory banks, GPU accelerator cards managing which becomes a tedious task for a user and a system administrator.
- Resource manager with in "slurm" tool helps to manage and represent resources to the users in a simplest way.

#### Job Schedular (SLURM)

Software

Components

- A scheduler checks the available resources within a cluster and manages which jobs run where and when.
- Allocating resources to each users for optimal utilization of system resources.
- Provides multiple algorithm, which provides different ways to initiate jobs on the resources.
- BACKFILL scheduling is the widely used and the most efficient algorithm.
- Provider batch jobs as well as Interactive jobs submission methods.

### NSM Clusters – Applications, Tools, Programming Models



S	<b>Bio-informatics</b>	MUMmer, HMM mpiBLAST, Clust	AER, MEME, PHYLIP,	Visualization Programs	GrADS, ParaView, Vislt, VMD	
ation	Molecular Dynamics	GPU), GROMAC	GPU), LAMMPS(CPU &	Dependency Libraries	NetCDF, PNETCDF, Jasper, HDF5, Tcl, Boost, FFTW	
Applic	Quantum Chemistry	Quantum-Espre NWChem,	esso, Abinit, CP2K,	Programming Models	MPI, OpenMP, OpenACC, CUDA, PGAS, Pthreads	
HPC /	Weather, Ocean, Climate	WRF, RegCM, N	3, 302 10M, ROMS	Additional applications, libraries, tools on different NSM systems		
	Disaster Management	ANUGA Hydro		as per r users of	equirements from respective systems	
		DL Frame work	: TensorFlow , keras, the	ano, pytorch, scikit-le	earn,scipy, cuDNN	
	AI/ ML/ DL	Data Science:	Numpy , RAPIDS			
	Tools/	Distributed DL	DL Framework: TensorFlow with Horovod			
	Technologies	Container Technology: enroot				
		JupyterHub:	DL application develop	ment platforms and w	veb based IDE	



### **Login Environment**

- The cluster can be accessed through 8 general login nodes.
- The login nodes is primary gateway to the rest of the cluster.
- All libraries, compilers, preinstalled applications, user installed application are available over login nodes.

### **Remote Login**

Accessing the

cluster

- You may access login node through ssh.
- Using SSH in Windows (Putty, Moab-xterm, etc).
- Using SSH in Linux via terminal.
- For example, to connect to the PARAM Ganga Login Node, with the username.
- Ex: ssh –p 4422 testuseruser@paramganga.iitr.ac.in

## **Access Policy**



- Access to Login nodes are in Round-Robin Mode.
- Users are not allowed to access Master/Management Nodes



One Vísíon. One Goal... Advanced Computing for Human Advancement...

### How to Access PARAM Ganga ?



- If you are using windows you can access via(SSH Clients):
  - MobaXterm
  - Putty, etc
- Within IIT Roorkee Campus:

ssh username@paramganga.iitr.ac.in

Outside IIT Roorkee Campus:

ssh <u>username@paramganga.iitr.ac.in</u> -p 4422

## **Ticketing Tool**



• A Support Portal will be created for Assisting the Users.

https://paramganga.iitr.ac.in/support



#### Frequently Asked Questions

Q Search

#### Q Search\_Your\_Queries





General FAQ	Q Search	Q Search_Your_Queries
	If your application is hybrid :	
Frequently Asked Questions	export I_MPI_FALLBACK="0" [Do not switch to other available network]	Table of contents
General FAQ	export I_MPI_FABRICS="shm:ofa"	How to get account on HPC cluster ?
Environment	<pre>export I_MPI_FABRICS="shm:dap1" (if using DAPL)</pre>	
Job Submission	For OpenMP :	How do I Access the HPC Cluster ?
Applications	<pre>export I_MPI_FABRICS="shm:shm"</pre>	What if, Error : Disk quota exceeded ?
ML/DL	To check which fabric is currently used, you can set the I_MPI_DEBUG environment variable to 2:	
Visualization	<pre>mpirun -np n -genv I_MPI_DEBUG=2 your_command/command_path; where "n" =&gt; number of</pre>	l get "Disk quota exceeded" erro message when trying to remove files. What can I do?
Best Practices	processes.	
Hardware Specifications	For Ex.: mpirun -np 48 -genv I_MPI_DEBUG=2 myprog	What if SCP not functional?
Help	You can also specify above variables in your mpirun command :	What if, Error : Out of memory / segmentation fault ?
Create New Ticket	<pre>mpirun -np n -genv I_MPI_FALLBACK=0 -genv I_MPI_FABRICS="shm:ofa"</pre>	
	your_command/command_path	What if, Error :ERROR : Bad Interpreter ?
	<pre>For Ex.: mpirun -np 48 -genv I_MPI_FALLBACK=0 -genv I_MPI_FABRICS="shm:ofa" myprog</pre>	
		Can I run MS Windows applications on HPC?
		How to Access Internet on HPC

Cannot find your queries ? Click here to create a ticket.

Next Environment →

How much of the file/space quota I have used ? Mv account expired ! What

Cluster ?

