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HIGH PERFORMANCE COMPUTING NEWSLETTER

INSTITUTE FOR PLASMA RESEARCH, GANDHINAGAR

Containers for HPC: The Future of Portable Scientific Workflows

High-Performance Computing (HPC) is evolving fast. Scientists and engineers today don't just need raw compute power - they need reproducibility, portability, and flexibility across different clusters, clouds, and supercomputers. This is where containers come in. By packaging software stack (application, libraries, compilers, dependencies) into a single image, user can:

- Ensure results are reproducible across clusters.
- Eliminate "it works on my system" issues.
- Move workloads easily between HPC centers and cloud platforms.
- Simplify deployment of complex software stacks.

While Docker dominates in DevOps, HPC Clusters typically uses Singularity/Apptainer, which is designed for multi-user HPC clusters: it runs containers without root privileges, integrates with schedulers (PBS, Slurm), and supports MPI and GPUs. In this two-part series, we'll go from beginner commands to a launch of containerized LAMMPS run with MPI and GPUs.

Part 1: Containers for HPC Beginners - 10 Commands You Must Know

This article highlights ten essential Singularity (Now Apptainer) commands that every HPC beginner should know. These commands form the foundation for pulling, running, and scaling containerized applications effectively within HPC workflows.

1) Check Version of Singularity installed

```
## Load the singularity module and verify the version
[user@login1 ~] $ module load singularity/3.5.3/3.5.3
[user@login1 ~] $ singularity --version
singularity version 3.5.3
```

2) Pull an Image

```
## After exporting proxy settings in environment, user may pull the image from any opensource repositories available (Here NGC catalog from nvidia is uses to pull images)
[user@login1 ~] $ singularity pull docker://nvcr.io/nvidia/base/ubuntu:20.04_x64_2022-09-23
INFO:    Converting OCI blobs to SIF format
WARNING: 'nodev' mount option set on /tmp, it could be a source of failure during build process
INFO:    Starting build...
Getting image source signatures
Copying blob fb0b3276a519 done
...
INFO:    Creating SIF file...
INFO:    Build complete: ubuntu_20.04_x64_2022-09-23.sif
```

3) Run a Container

```
## Start the container using the default command defined in the image (like bash or an application)
[user@login1 ~] $ singularity run ubuntu_20.04_x64_2022-09-23.sif
Singularity>
```

4) Execute a Command Inside

```
## Execute command directly from image using exec command with singularity
[user@login1 ~] $ singularity exec ubuntu_20.04_x64_2022-09-23.sif cat /etc/os-release
NAME="Ubuntu"
VERSION="20.04.5 LTS (Focal Fossa)"
```

5) Shell Into a Container

```
## Get an interactive shell inside the container — useful for debugging and exploring environments
[user@login1 ~] $ singularity shell ubuntu_20.04_x64_2022-09-23.sif
Singularity>
```

6) Bind Host Directories

```
## Mount host directories (like scratch or Home folders) inside container
[user@login1 ~] $ singularity exec --bind /scratch/scratch_data/shivam.patel:/data ubuntu_20.04_x64_2022-09-23.sif ls /data
Programs  comsol  demo  source  sys_info.sh
```

7) Enable GPU Support

```
## Expose GPUs to your container (required for CUDA, TensorFlow, PyTorch, etc.).
[user@gn01 ~] $ singularity exec --nv tensorflow.sif python detect_gpu.py
>>> import tensorflow as tf; physical_devices = tf.config.list_physical_devices('GPU'); print("Physical devices:", physical_devices)
Physical devices: [PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU'), PhysicalDevice(name='/physical_device:GPU:1', device_type='GPU')]
```

8) Run MPI Applications

```
## Use MPI from the host with Singularity — essential for multi-node parallel HPC jobs.
[user@cn001 ~] $ singularity exec lammps_stable_22Jul2025.sif mpirun -np 2 hostname
cn001
cn001
```

9) Inspect the Container

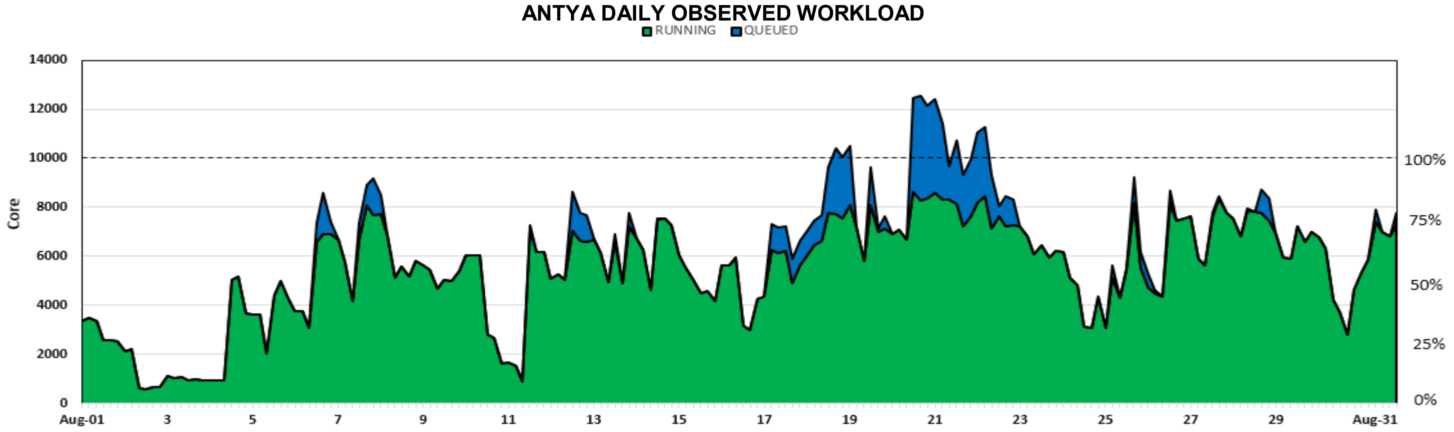
```
## See metadata like labels, environment variables, and image details.
[user@login1 ~] $ singularity inspect lammps_stable_22Jul2025.sif
org.label-schema.build-date: Monday_1_September_2025_14:52:18_IST
org.label-schema.schema-version: 1.0
org.label-schema.usage.singularity.deffile.bootstrap: docker
org.label-schema.usage.singularity.deffile.from: nvcr.io/nvidia/lammps:stable_22Jul2025
org.label-schema.usage.singularity.version: 3.5.3
```

10) Build Your Own Image

```
## Convert a definition file into a container image (usually done on a Local PC, then moved to HPC).
[user@local_pc ~] $ cat openmpi.def
Bootstrap: library
From: ubuntu:22.04
%post
   export DEBIAN_FRONTEND=noninteractive
   ln -fs /usr/share/zoneinfo/Asia/Kolkata /etc/localtime
   echo "Asia/Kolkata" > /etc/timezone
   apt update && apt install -y build-essential wget tzdata
   wget https://download.open-mpi.org/release/open-mpi/v4.1/openmpi-4.1.5.tar.gz
   tar -xzf openmpi-4.1.5.tar.gz
   cd openmpi-4.1.5
   ./configure --prefix=/usr/local/openmpi --enable-mca-no-build=btl-uct --enable-mca-no-build=op-avx --enable-mpi-thread-multiple --enable-mpi1-compatibility
   make -j8
   make install
%environment
   export PATH=/usr/local/openmpi/bin:$PATH
   export LD_LIBRARY_PATH=/usr/local/openmpi/lib:$LD_LIBRARY_PATH
   export LD_RUN_PATH=/usr/local/openmpi/lib:${LD_RUN_PATH}
   export PKG_CONFIG_PATH=/usr/local/openmpi/lib/pkgconfig:${PKG_CONFIG_PATH}
   export CPATH=/usr/local/openmpi/include:${CPATH}
%labels
   Maintainer "Shivam Patel"
   Description "Singularity container for Openmpi with GLIBC 2.27"
[user@local_pc ~] $ singularity build --fakeroot openmpi.sif openmpi.def
INFO:    Starting build...
INFO:    Verifying bootstrap image /home/shivam.patel/.singularity/cache/library/sha256.7a63c14842a5c9b9c0567c1530af87afbb82187444ea45fd7473726ca31a598b
INFO:    Running post scriptlet
+ export DEBIAN_FRONTEND=noninteractive
+ ln -fs /usr/share/zoneinfo/Asia/Kolkata /etc/localtime
+ echo Asia/Kolkata
+ apt update
...
```

With these 10 commands, user can pull, run, debug, and scale containerized applications on HPC system. In Part 2, these commands will be used with a real-world example: running the LAMMPS (compatible with CUDA 11.2 version) molecular dynamics package from NVIDIA's NGC catalog in a multi-node, multi-GPU PBS job using singularity.

ANTYA Utilization: AUGUST 2025



ANTYA HPC Users' Statistics August 2025

Total Successful Jobs~ 1843

> Top Users (Cumulative Resources)

- **CPU Cores** Sagar Choudhary
- **GPU Cards** Gaurav Garg
- **Walltime** Sagar Choudhary
- **Jobs** Jugal Chowdhury

ANTYA Usage, Updates and News

- **Scheduled Downtime**: There was no downtime of ANTYA for August 2025.
- **Job Submissions**: The highest job loads were observed in the *regularq*, *mediumq*, *serialq*, *longq and ansysq* queues, reflecting sustained user activity across multiple workloads in various queues.
- **Cluster Utilization**: The system maintained an average utilization of ~54.76% and peak utilisation of ~86.19%.

Packages/Applications Installed: No new modules have been installed this month. To view list of available modules.
> module avail

Other Recent Work on HPC

Influence of convective and radiative heat transfer on effective thermal conductivity of Solid Breeder pebble beds using DEM-CFD simulations	Deepak Sharma
Confinement-driven structural transitions in a dusty plasma crystal	Sushree Monalisha Sahu
Simulation Studies of Resonant Excitation of Electron Bernstein Waves in Capacitive Discharges	Sarveshwar Sharma
Development of Nondestructive techniques for Gas cooled Plasma Facing Components	Kedar Satish Bhope
Electron Bernstein Waves in Magnetized Capacitive Discharges: First Simulation-Based Evidence and Associated Plasma Dynamics	Sarveshwar Sharma
Design and Application of a Quasi-Optical Notch Filter for Mitigating RF Stray Radiation in the ITER ECE Diagnostic System	Suman Danani
Generating Nanosecond Pulse Electric Field using RF transmission line and Semiconductor devices	Supriya Anil Nair
A Study of Intermittent Ion Beam Irradiation with Continuous Temperature Variation on Silicon Surface Nanopatterning	Dr. Rakhi

Acknowledgement

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Join the HPC Users Community

hpcusers@ipr.res.in

If you wish to contribute an article in GAṆANAM, please write to us.

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Contact us

HPC Team (*hpcteam@ipr.res.in*)

Computer Division, IPR