NVIDIA DGX SuperPOD

User Guide

Featuring NVIDIA DGX A100 Systems

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Document History

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1. NVIDIA DGX SuperPOD Overview

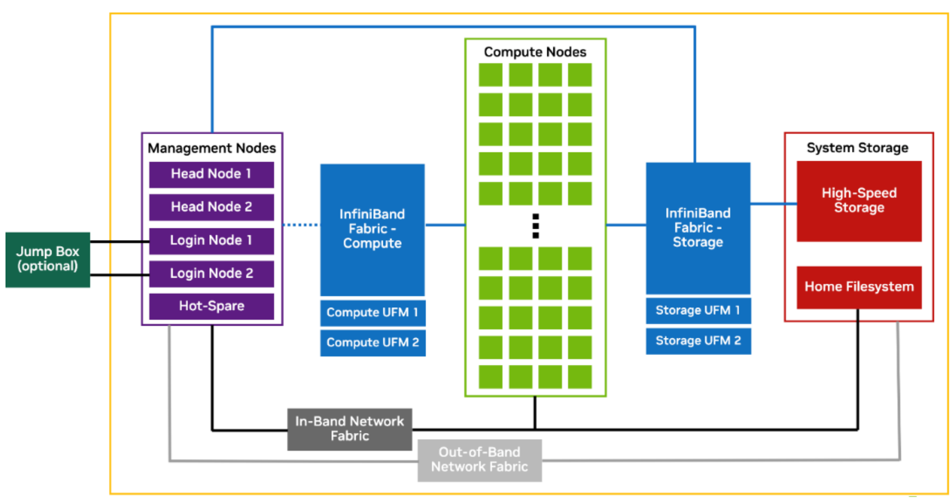
The NVIDIA DGX SuperPOD™ is a multi-user system designed to run large artificial intelligence (AI) and high-performance computing (HPC) applications efficiently. While the system is composed of many different components, it should be thought of as a single system that can manage simultaneous use by many users and provide advanced access controls for queuing and scheduling resources. This ensures maximum performance, provides the tools for collaboration between users, and security controls to protect data and limit user interaction where necessary.

This document does not cover information about the DGX SuperPOD that is specific to local policies or general Unix/Linux topics such access, queuing, quotas, compiling, and editing and manipulating files and data.

1.1 Logical System Diagram

Figure 1 provides a logical depiction of the DGX SuperPOD and all the components that enable it to work as a single multi-user, system.

Figure 1. Logical depiction of the DGX SuperPOD



The boxes and connections Figure 1 indicate that these components are not a part of the user-experience. Any lines that are dotted indicate that there is some connectivity between the two resources, but not necessarily every sub-component is connected. The optional jump box is an optional component outside of the DGX SuperPOD that enables remote access into it.

Components from Figure 1 are further described in Table 1.

Table 1. DGX SuperPOD components

Component	Description
Jump Box/Entry Point	The Jump Box/Entry Point is the gateway into the DGX SuperPOD intended to provide a single-entry point into the cluster and additional security when required. It is not actually apart of the DGX SuperPOD, but of the corporate IT environment. This function is defined by local IT requirements.
Login Nodes	The login nodes are the entry point for the user into the DGX SuperPOD. A login node is a CPU-only node for light-weight tasks where the user can develop code, submit, and monitor jobs, and manage your data.
Compute Nodes	The compute nodes are where the user work gets done on the system. Each compute node is an individual server, but with the high-speed fabric, applications can be efficiently spread out across multi-nodes.
High-Speed Storage	High-speed storage is optimized for efficient reading and writing of large data files. The high-speed storage is often treated as scratch, as it is difficult or impossible to back-up all data stored on the system. This is where datasets, checkpoints, and other large files should be stored.
Home File System	The home file system is traditional highly reliable network file system that trades performance for stability and enterprise management features. The assigned space is generally smaller than what is available on high-speed storage. Users should store scripts, code, Dockerfiles, and other small and important files.
InfiniBand Fabric—Compute	The Compute InfiniBand Fabric is the high-speed network fabric connecting all the compute nodes together to enable high-bandwidth and low-latency communication between the compute nodes.
InfiniBand Fabric—Storage	The Storage InfiniBand Fabric is the high-speed network fabric dedicated for storage traffic. Storage traffic is dedicated to its own fabric to remove interference with the node-to-node application traffic that can degrade overall performance.
In-band Network Fabric	The In-band Network Fabric provides fast Ethernet connectivity between all the node in the DGX SuperPOD. While its use should be transparent to the users, it hosts important traffic for node management and home file system access.

1.2 Navigating the DGX SuperPOD

When a user first logs into the DGX SuperPOD, it will look like any other Linux system. They will be placed into their home directory and standard Linux commands will work.

For example:

```
# pwd
/home/dgxuser
# ls -al
./bashrc
```

In addition, the high-speed file system will be available on the login nodes and all the compute nodes:

```
# ls /lustre/fs1/
projects
```

The DGX SuperPOD is a collection of nodes and access is managed through the workload management system. The default workload management system is Slurm. Slurm enables submitting and managing jobs. See Workload Management for more details.

> **Note:** The description regarding accessing the DGX SuperPOD is the default way of using the command line to interact with the system. Local deployments may provide other user interfaces for interacting with the system. In addition, the examples in this document use a standard naming convention for system names and directories but may be changed for a given environment.

2. Workload Management

2.1 Introduction

Workload management is the submission and control of work on the system. Slurm is the workload management system used. Slurm is an open-source job scheduling system for Linux clusters, most frequently used for HPC applications. This guide covers some of the basics to get started using Slurm as a user on the DGX SuperPOD, including how to use Slurm commands such as `sinfo`, `srun`, `sbatch`, `squeue`, and `scancel`.

The basic flow of a workload management system is the user submits a job to the queue. A job is a collection of work to be executed. Shell scripts are the most common because a job often consists of many different commands.

The system will take all the jobs submitted that are not yet running, look at the state of the system, and then map those jobs to the available resources. This workflow enables users to manage their work within large groups with the system determining the optimal way to order jobs for maximum system utilization (or other metrics that system administrators can configure).

2.2 Viewing System State

To see all nodes in the cluster and their current state, ssh to the Slurm login node for your cluster and run the `sinfo` command:

```
$ sinfo
PARTITION    AVAIL        TIMELIMIT    NODES        STATE        NODELIST
batch*       up           infinite     9            idle         dgx[1-9]
```

There are nine nodes available in this example, all in an idle state. If a node is busy, its state will change from `idle` to `alloc` when the node is in use:

```
$ sinfo
PARTITION    AVAIL        TIMELIMIT    NODES        STATE        NODELIST
batch*       up           infinite     1            alloc        dgx1
batch*       up           infinite     8            idle         dgx[2-9]
```

2.3 Running Jobs

There are three ways to run jobs under Slurm. Jobs can be run with `sbatch`, where the work is queued in the system and control is returned to the prompt. The second is with `srun`, which will run the job on the system and the command will block while it waits to run and then runs to completion. The third way is to submit interactive jobs where `srun` is used to create the job, but shell access is given.

2.3.1 Running Jobs with `sbatch`

While the `srun` command blocks any other execution in the terminal, `sbatch` can be run to queue a job for execution when resources are available in the cluster. Also, a batch job will enable several jobs to queue up and run as nodes become available. It is therefore good practice to encapsulate everything that needs to be run into a script and then execute with `sbatch`.

```
$ cat script.sh
#!/bin/bash
/bin/hostname sleep 30

$ sbatch script.sh
2322
$ squeue
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
 2322   batch     script.sh  user  R       0:00     1    dgx1
$ ls
slurm-2322.out
$ cat slurm-2322.out
dgx1
```

2.3.2 Running Jobs with `srun`

To run a job, use the `srun` command:

```
$ srun hostname
dgx1
```

This instructed Slurm to find the first available node and run `hostname` on it. It returned the result in our command prompt. It is just as easy to run a different command that runs a python script or a container using `srun`.

Sometimes it is necessary to run on multiple systems:

```
$ srun --ntasks 2 -l hostname
dgx1
dgx2
```

2.3.3 Running Interactive Jobs with `srun`

When developing and experimenting, it is helpful to run an interactive job, which requests a resource and provides a command prompt as an interface to it:

```
slurm-login:~$ srun --pty /bin/bash
dgx1:~$ hostname
dgx1
dgx1:~$ exit
```

During interactive mode, the resource is being reserved for use until the prompt is exited. Commands can be run in succession.

Before starting an interactive session with `srun`, it may be helpful to create a session on the login node with a tool like `tmux` or `screen`. This will prevent a user from losing interactive jobs if there is a network outage or the terminal is closed.

> **Note:** Local administrative policies may restrict or prevent interactive jobs. Ask a local system administrator for specific information about running interactive jobs.

2.4 Specifying Resources when Submitting Jobs

When submitting a job with `srun` or `sbatch`, request the specific resources needed for the job. Allocations are all based on tasks. A task is a unit of execution. Multiple GPUs, CPUs, or other resources can be associated to a task. A task cannot span a node. A single task or multiple tasks can be assigned to a node.

As shown in Table 2 Resources can be requested several different ways.

Table 2. Methods to specify `sbatch` and `srun` options

`sbatch/srun` Option	Description
`-N, --nodes=`	Specify the total number of nodes to request
`-n, --ntasks=`	Specify the total number of tasks to request
`--ntasks-per-node=`	Specify the number of tasks per node
`-G, --gpus=`	Total number of GPUs to allocate for the job
`--gpus-per-task=`	Number of GPUs per task
`--gpus-per-node=`	Number of GPUs to be allocated per node
`--exclusive`	Guarantee that nodes are not shared among jobs

While there are many combinations of options, here are a few common ways to submit jobs:

Request two tasks:

```
srun -n 2 <cmd>
```

Request two nodes, eight tasks per node, and one GPU per task:

```
sbatch -N 2 --ntasks-per-node=8 --gpus-per-task=1 <cmd>
```

Request 16 nodes, eight GPUs per node:

```
sbatch -N 16 --gpus-per-node=8 --exclusive <cmd>
```

2.5 Monitoring Jobs

To see which jobs are running in the cluster, use the `squeue` command:

```
$ squeue -a -l
Tue Nov 17 19:08:18 2020
JOBID PARTITION NAME USER STATE TIME TIME_LIMIT NODES NODELIST(REASON)
9      batch    bash user01 RUNNING 5:43 UNLIMITED 1 dgx1
10     batch    Bash user02 RUNNING 6:33 UNLIMITED 2 dgx[2-3]
To see just the running jobs for a particular user USERNAME:
$ squeue -l -u USERNAME
```

The `squeue` command has many different options available. See the man page for more details.

2.6 Canceling Jobs

To cancel a job, use the `scancel` command:

```
$ scancel JOBID
```

2.7 Additional Resources

Additional resources include:

- SchedMD Slurm Quickstart Guide
- LLNL Slurm Quickstart Guide
- https://github.com/NVIDIA/deepops/blob/master/docs/slurm-cluster/slurm-usage.md

3. Using Containers

Containers provide a way to encapsulate all the software dependencies of an application and enable it to be deployed on different systems. Containers are the preferred way to run applications on the DGX SuperPOD.

The DGX SuperPOD is deployed with two tools, Pyxis and Enroot, to help simplify the secure use of containers on the DGX SuperPOD. Pyxis extends the functionality of Slurm so that jobs can be launched directly into a container with `srun`. Enroot is a light-weight container-runtime that enables traditional container images to be run in unprivileged mode.

3.1 Examples

Here are some example commands for working with user containers:

> Submit a job to Slurm on a worker node.

```
$ srun grep PRETTY /etc/os-release
PRETTY_NAME="Ubuntu 20.04.4 LTS"
```

> Submit a job to Slurm and launching it in a container.

The `--container-image` option is used to specify which container to use.

```
$ srun --container-image=centos grep PRETTY /etc/os-release
PRETTY_NAME="CentOS Linux 7 (Core)"
```

> Mount a file from the host and run the command on it from inside the container.

```
$ srun --container-image=nvcr.io/nvidia/pytorch:22.12-py3 --container-mounts=/etc/os-release:/host/os-release grep PRETTY /host/os-release
pyxis: importing docker image: nvcr.io/nvidia/pytorch:22.12-py3
pyxis: imported docker image: nvcr.io/nvidia/pytorch:22.12-py3
PRETTY_NAME="Ubuntu 20.04.4 LTS"
```

> The `--container-mounts` option can be used to mount both files and directories into the container environment. Multiple options should be separated by commas.

```
$ srun -N 2 --ntasks-per-node=1 --container-image=nvcr.io/nvidia/pytorch:22.12-py3 --container-mounts=/etc/os-release:/host/os-release grep PRETTY /host/os-release
pyxis: imported docker image: nvcr.io/nvidia/pytorch:22.12-py3
pyxis: imported docker image: nvcr.io/nvidia/pytorch:22.12-py3
```

- Submit the same command across two nodes, mounting the current directory as `/work` in the container.

  The full network name of the container is different. Enroot requires the separator between the network repository name (`nvcr.io` in this case) to be separated by a `#`, not a slash (`/`).

```
srun -N 2 --ntasks-per-node=1 \
--container-image=nvcr.io/nvidia/pytorch:22.12-py3 --container-
mounts=$(pwd):/work \
/bin/bash -c 'uname -n && cat /etc/os-release | grep PRETTY_NAME'
dgx1
PRETTY_NAME="Ubuntu 20.04.5 LTS"
dgx2
PRETTY_NAME="Ubuntu 20.04.5 LTS"
```

Further resources are available at these links:

- For a tutorial on running a multi-node Pyxis/Enroot BERT container, see this guide.
- For a hello world tutorial on using MPI to run multi-gpu and multi-node jobs, see this guide.
- For a tutorial on running a multi-node machine learning job using Dask on Slurm, see this guide.

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