

NVIDIA DGX SuperPOD: IBM Storage Scale and IBM 3500

Reference Architecture

Featuring NVIDIA DGX H100 and A100 Systems

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Abstract

The <u>NVIDIA DGX SuperPOD[™]</u> with <u>NVIDIA DGX[™] H100</u> or <u>NVIDIA DGX A100</u> systems is an artificial intelligence (AI) supercomputing infrastructure, which provides the computational power necessary to train today's state-of-the-art deep learning (DL) models and to fuel future innovation. The DGX SuperPOD delivers groundbreaking performance, deploys as a fully integrated system, and is designed to solve the world's most challenging computational problems.

This DGX SuperPOD reference architecture (RA) is the result of collaboration between DL scientists, application performance engineers, and system architects to build a system capable of supporting the widest range of DL workloads. The performance delivered by the DGX SuperPOD with DGX systems enables the rapid training of DL models at great scale. The integrated approach of provisioning, management, compute, networking, and fast storage enables a diverse, multi-tenant system that can span data analytics, model development, and Al inference.

In this paper, the <u>IBM Storage Scale System 3500</u> was evaluated for suitability in supporting DL workloads when connected to the DGX SuperPOD. IBM 3500 is a modern implementation of software-defined storage with low latency NVMe physical storage, advanced erasure coding, connected using InfiniBand and Ethernet networking. Multiple IBM 3500 systems can be aggregated to create a high-performance cluster filesystem, tiered for data economics, or connected to multiple clusters for geographic and cross platform data sharing in a single global data platform. The IBM 3500 is a 2U building block that makes it easy to deploy, manage, and grow fast storage for AI with NVIDIA DGX systems.

The DGX SuperPOD is a turnkey solution validated at scale with scale-out IBM 3500 network attached storage (NAS) systems. Joint testing and integration ensure the NVIDIA DGX SuperPOD is a rapidly deployed and a robust solution for scalable AI development. NVIDIA and IBM jointly test, plan, and install the system, with the storage backed by IBM global deployment and support services.

As configured, tested, and deployed in the NVIDIA SuperPOD, IBM 3500 systems can be used for all DL workloads including:

- > Training models efficiently with directly from IBM Storage Scale.
- > Automatically leverage local resources as cache to minimizing rereading data across the network.
- > Workspace for long-term storage (LTS) of datasets.
- A centralized repository for the acquisition, manipulation and sharing of results using standard protocols like NFS, SMB, and S3.

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Storage Overview

Training performance can be limited by the rate at which data can be read and reread from storage. The key to performance is the ability to read data multiple times, ideally from local storage. The closer the data is cached to the GPU, the faster it can be read. Storage must be designed considering the hierarchy of different storage technologies, either persistent or nonpersistent, to balance the needs of performance, capacity, and cost.

Storage Caching Hierarchy

The storage caching hierarchy of the DGX system is shown in Table 1. Depending on data size and performance needs, each tier of the hierarchy can be leveraged to maximize application performance.

| Storage Hierarchy Level | Technology | Total Capacity ¹ | Performance ¹ | | | |
|--|------------|-------------------------------|--------------------------|--|--|--|
| RAM | DDR4 | 2 TB per system ² | > 200 GB/s | | | |
| Internal Storage | NVMe | 30 TB per system ³ | > 50 GB/s | | | |
| Total capacity and performance values are per system. Shared between the operating system, application, and other system processes PCIe Gen 4 NVMe SSD storage | | | | | | |

Table 1. DGX system storage and caching hierarchy

Caching data in local RAM provides the best performance for reads. This caching is transparent after the data is read from the filesystem.

While local storage is fast, it is not practical to manage a dynamic environment with local disk alone in multi-node environment. Functionally, centralized storage can be as quick as local storage on many workloads.

Storage Performance Requirements

Performance requirements for high-speed storage greatly depend on the types of Al models and data formats to be used. The DGX SuperPOD has been designed as a capability-class system that can manage any workload both today and in the future. However, if systems are going to focus on a specific workload, such as natural language processing (NLP), it may be possible to better estimate performance needs of the storage system.

To enable customers to characterize their own performance requirements, some general guidance on common workloads and datasets is shown Table 2.

| Storage Performance Level Required | Example Workloads | Dataset Size |
|---------------------------------------|---|--|
| Good | NLP | Most all datasets fit in cache |
| Better | Image processing with compressed images, ImageNet/ResNet-50 | Many to most datasets can fit within the local system's cache. |
| Best | Training with 1080p, 4K, or uncompressed images, offline inference, ETL | Datasets are too large to fit into cache, massive first epoch I/O requirements, workflows that only read the dataset once |

Table 2. Characterizing different I/O workloads

Performance estimates for the storage system necessary to meet the guidelines in Table 2 are in:

- <u>Table 4</u> of the NVIDIA DGX SuperPOD Reference Architecture—DGX H100 Systems.
- <u>Table 8</u> of the NVIDIA DGX SuperPOD Reference Architecture—DGX A 100 Systems.

Achieving these performance characteristics may require the use of optimized file formats such as TFRecord, RecordIO, or HDF5.

The high-speed storage provides a shared view of an organization's data to all systems. It needs to be optimized for small, random I/O patterns, and provide high peak system performance and high aggregate filesystem performance to meet the variety of workloads an organization may encounter.

About the IBM Storage Scale System 3500

The IBM Storage Scale System 3500, shown in Figure 1, combines the performance of NVMe storage technologies with the reliability and the rich features of <u>IBM Storage</u> <u>Scale</u> in a powerful 2U storage system that scales out for performance and capacity.

Figure 1. IBM Storage Scale System 3500



<u>IBM Storage Scale</u> on NVMe is designed to be the market leader in all-flash performance, and scalability with read performance of up to 125 GB/s and 1.3 million IOPs per NVMe all-flash appliance. Providing data-driven multicloud storage capacity, the NVMe all-flash appliance is deeply integrated with the software-defined capabilities of IBM Storage Scale to seamlessly plug it into for analytics, scalable cluster, or Al workload.

Available with multiple drive options and advanced erasure coding, the IBM 3500 provides options to optimize costs for different installation sizes. As with all IBM Storage Scale solutions, capacity and performance can be scaled and tiered. Combining IBM 3500 all-NVMe systems provides nearly linear performance scalability. IBM 3500 solutions may also be used as an all-flash NVMe performance tier on slower storage, including tape or object storage.

IBM Storage Scale is an industry leader in high-performance file systems. The underlying general parallel file system (GPFS) provides scalable throughput and low-latency data access, as well as superior metadata performance. Unlike other systems that can easily bottleneck, the distributed architecture of a parallel filesystem provides reliable performance for multi-user sequential and random read or write. This is particularly important in AI clusters where multiple compute nodes may need to read or write to the same file. IBM Storage Scale has been proven on the largest AI clusters in the world, including the US National Labs supercomputers Summit and Sierra, as well as the Circe supercomputer built by NVIDIA.

IBM Storage Scale provides Container Native Access and Operators to support Kubernetes driven DevOps and Data Ops practices. In addition, IBM Storage Scale provides enterprise features such as call-home proactive support, encryption, and audit file logging that works with enterprise <u>security information and event management</u> (<u>SEIM</u>) platforms.

Validation Methodology and Results

Three classes of validation tests are used to evaluate a particular storage technology and configuration for use with the DGX SuperPOD: microbenchmark performance, real application performance, and functional testing. The microbenchmarks measure key I/O patterns for DL training and are crafted so they can be run on nodes with CPU only. This reduces the need for large GPU-based systems to validate storage. Real DL training applications are then run on a DGX SuperPOD to confirm that the applications meet expected performance. Beyond performance, storage solutions are evaluated for robustness and resiliency as part of functional testing.

The NVIDIA DGX SuperPOD storage validation process leverages a "Pass or Fail" methodology. Specific targets are set for the microbenchmark test. Each benchmark result is graded as good, fair, or poor. A passing grade is one where at least 80% of the tests are good, and none are poor. In addition, there must be no catastrophic issues created during testing. For application testing, a passing grade is one where all cases complete within 5% of the roofline performance set by running the same tests with data staged on the DGX RAID. For functional testing, a passing grade is one where all functional tests meet their expected outcomes.

Microbenchmarks

In the Storage Performance Requirements section, there are several high-level performance metrics that storage systems must meet to qualify as a DGX SuperPOD solution. Current testing requires that solutions meet the "Best" criteria discussed in the table. In addition to these high-level metrics, several groups of tests are run to validate the overall capabilities of the proposed solutions. These include single-node tests where the number of threads is varied and multi-node tests where a single thread count is used and as the number of nodes vary. In addition, each test run in both Buffered and DirectIO modes and when I/O is performed to separate files or when all threads and nodes operate on the same file.

Four different read patterns are run. The first read operation is sequential where no data is in the cache. The second read operation is executed immediately thereafter to evaluate the ability for the filesystem to cache data. The cache is purged and then the data is read again, this time randomly. Lastly, the data is reread again randomly, to evaluate data caching.

IOR benchmark for single-node and multi-node tests was used.

Hero Benchmark Performance

The hero benchmark helps establish the peak performance capability of the entire solution. Storage parameters, such as filesystem settings, I/O size, and controlling CPU affinity, were tuned to achieve the best read and write performance. Storage devices were expected to demonstrate that quoted performance was close to measured performance. Other tests are crafted to demonstrate performance of real workloads.

The delivered solution for a single SU had to demonstrate over 20 GiB/s for writes and 65 GiB/s for reads. Ideally, the write performance should be at least 50% of the read performance. However, some storage architectures have a different balance between read and write performance, so this is only a guideline and read performance is more important than write.

Single-Node, Multi-File Performance

For single-node performance, I/O read and write performance is measured by varying the number of threads in incremental steps. Each thread writes (and reads) to (and from) its own file in the same directory.

For single-node performance tests, the number of threads is varied from 1 to the ideal number of threads to maximize performance—typically more than half the cores (64), but no more than the total physical cores (128). The I/O size is varied between 128 KiB and 1 MiB and the tests are run with Buffered I/O and Direct I/O.

The target performance for these tests is shown in Table 3.

| Thread | Buffered or | I/O size | Performance | | | | |
|--------|-------------|----------|-------------|-------|--------|----------------|------------------|
| Count | DirectIO | (KiB) | Write | Read | Reread | Random Read | Random Reread |
| 1 | Buffered | 128 | 512 | 1,024 | 1,536 | 256 | 1,536 |
| 1 | Buffered | 1024 | 800 | 3,072 | 4,608 | 768 | 1,024 |
| 1 | Direct | 1024 | 1,024 | 1,024 | - | 1,024 | - |

Table 3. Single-node, multi-file performance targets

When maximizing single-node performance, the thread count may vary, however it is expected that performance does not drop significantly when additional threads are used beyond the optimal thread count.

Target performance for single-node performance with multiple threads is in Table 4. The optimal number of threads may vary for any storage configuration.

| Thread | Buffered or I/O siz DirectIO (KiB) | I/O size | Performance | | | | |
|--------|---------------------------------------|----------|-------------|--------|--------|----------------|------------------|
| Count | | (KiB) | Write | Read | Reread | Random Read | Random Reread |
| | Buffered | 128 | 8,000 | 12,000 | 18,000 | 12,000 | 18,000 |
| Varies | Direct | 128 | 8,000 | 15,000 | - | 15,000 | - |
| | Buffered | 1024 | 10,000 | 20,000 | 30,000 | 20,000 | 30,000 |
| | Direct | 1024 | 10,000 | 20,000 | - | 20,000 | - |

Table 4. Single-node, multi-threaded performance targets

Reread performance relative to read performance can vary substantially between different storage solutions. The reread performance should be at least 50% of the read performance for both sequential and random reads.

Multi-Node, Multi-File Performance

The next test performed is multi-node I/O read and write test to make sure that the storage appliance can provide the minimum required buffered read and write per system for the DGX SuperPOD. This benchmark determines the capacity of a filesystem to scale performance of different I/O patterns. Performance should scale linearly from one to a few nodes, reach a maximum performance, then not drop off significantly as more nodes are added to the job.

The target performance for a single SU of 20 nodes is 65 GiB/s for reads with I/O size of 128 KiB or 1,024 KiB, and if the I/O is Direct or Buffered. The write performance should be at least 20 GiB/s, but ideally it would be 50% of the read performance. Results from these tests must be interpreted carefully as it is possible to add more hardware to achieve these levels. Overall performance is the goal, but it is desirable that the performance comes from an efficient architecture that is not over-designed for its use.

Single-File I/O Performance

A key I/O pattern is reading data from a single file. Often the fastest way to read data is when all the data is organized into a single file, such as the RecordIO format. This can often be the fastest way to read data because it eliminates any of the open and close operations required when data are organized into multiple large files. Single-file reads are a key I/O pattern on DGX SuperPOD configurations.

Targeted performance and expected I/O behavior is that the single-node, multi-threaded, writes can successfully create the file, that sequential read and random read performance is good, and that read performance scales as more nodes are used. Multi-node, multi-threaded, single file writes are not evaluated. In addition, it is expected that buffered reread performance will be like the multi-file reread performance. Target performance for single file I/O is in Table 5.

| Node Count | Buffered or | I/O size | | Performance | | | | |
|---------------|-------------|----------|--------|---------------------|----------------|-------------------------------|--|--|
| | DirectIO | (KiB) | Read | Reread ¹ | Random Read | Random Reread ¹ | | |
| 1 | Buffered | 128 | 2,500 | 1 | 2,500 | 1 | | |
| 1 | Direct | 128 | 15,000 | - | 15,000 | - | | |
| 1 | Buffered | 1024 | 3,000 | 1 | 3.000 | 1 | | |
| 1 | Direct | 1024 | 20,000 | - | 20,000 | - | | |
| 20 | Buffered | 128 | 65,000 | 1 | 65,000 | 1 | | |
| 20 | Direct | 128 | 65,000 | - | 65,000 | - | | |
| 20 | Buffered | 1024 | 65,000 | 1 | 65,000 | 1 | | |
| 20 | Direct | 1024 | 65,000 | - | 65,000 | - | | |

 Table 5. Single-file read performance targets

Application Testing

Microbenchmarks provide indications of the peak performance of key metrics. However, it is application performance that is most important. A subset of the MLPerf Training benchmarks is used to validate storage performance and function. Here, both single-node and multi-node configurations are evaluated to ensure that the filesystem can support different I/O patterns and workloads. Training performance when data is staged on the DGX RAID was used as the baseline for performance. The performance goal is for the total time to train when data is staged on the shared filesystem to be within 5% of those measured when data is staged on the local RAID. This is not just for individual runs, but also when multiple cases are run across the DGX SuperPOD at the same time.

ResNet-50

ResNet-50 is the canonical image classification benchmark. Its dataset size is over 100 GiB and it has a requirement for fast data ingestion. On a DGX system, a single node training requires approximately 3 GiB per second and the dataset is small enough that it can fit into cache. Preprocessing can vary, but the typical image size is approximately 128 KiB. One challenge of this benchmark is that at NVIDIA the processed images are stored in the RecordIO format (i.e. one large file for the entire dataset) because this provides the best performance for MLPerf. This one large file can stress shared filesystem architectures that do not distribute the data across multiple targets or controllers.

NLP-BERT

BERT is the reference standard NLP model. In this test, the system is filled with two eight node jobs and four single node jobs (or less if not all nodes of the SU are available). It is expected that the total time to train is within 5% of that measured when training from the local raid. This test does not stress the filesystem but does ensure that local caching is operating as needed.

Recommender—DLRM

The recommender model has different training characteristics than ResNet-50 and BERT in that the model trains in less than a single epoch. This means that the data set is read no more than once, and local caching of data cannot be used. To achieve full training performance, DLRM must be able to read data at over 6 GiB/s. In addition, the file reader uses DirectIO that stresses the filesystem differently than the other two files. The data are formatted into a single file.

This test is only run as a single node test; however, several tests are run where the number of simultaneous jobs vary from one to the total number of nodes available. It is expected that the shared filesystem only sustains performance up to the peak performance measured from the hero test.

For 20 simultaneously cases, the storage system would have to provide of over 120 GiB/s of sustained read performance, more than what is prescribed in the Storage Performance Requirements section. Even the best performance outlined in that section is not meant to support every possible workload. It is meant to provide a balance of high throughput while not over-architecting the system.

Summary

NVIDIA evaluations show that the IBM Storage Scale System 3500 with Storage Scale file system meets the DGX SuperPOD performance and functionality requirements. It is a great choice to pair with a DGX SuperPOD to meet current and future storage needs.

As storage requirements grow, IBM 3500 building blocks can be added to seamlessly scale capacity, performance, and capability. The combination of NVME hardware and IBM Storage Scale parallel file system architecture provides excellent random read performance, often just as fast as sequential read patterns. Testing has validated that each IBM 3500 can deliver the highest levels of per node performance and meet all our application performance requirements. The IBM Storage Scale parallel file system provides a platform that is fully supported with the NVIDIA DGX SuperPOD and has been deployed in production.

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