IBM Storage Reference Architecture with NVIDIA DGX A100 Systems

Version 1 Release 1

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Content

About this document

This document is intended to facilitate the deployment and configuration of the NVIDIA DGX™ A100 systems using IBM Spectrum Scale and IBM Elastic Storage System (ESS) 3000. It is the latest in the series of IBM and NVIDIA DGX Reference Architectures for each generation of NVIDIA DGX systems.

The information in this document is distributed on an "as is" basis without any warranty that is either expressed or implied. Support assistance for the use of this material is limited to situations where IBM Spectrum Scale® and/or IBM ESS 3000 are supported and entitled and where the issues are specific to a blueprint implementation.

Scope

This blueprint guide provides a solutions architecture and related solution configuration parameters with the following essential components:

- IBM Spectrum Scale
- IBM Elastic Storage System 3000
- NVIDIA DGX A100 Systems
- NVIDIA InfiniBand (IB) Switches

This blueprint does not:

- Replace any official manuals and documents issued by IBM
- Replace any official manuals and documents issued by NVIDIA

The NVIDIA DGX POD™ with IBM storage reference architecture does not describe data and metadata integration of data ingest, pre-processing, archiving, tiering, and legacy data stores. Though these use-cases are supported by IBM Spectrum Scale, describing them is not in the scope of this document.

Prerequisites

This technical paper assumes the following prerequisites:

- Basic knowledge of IBM Elastic Storage Server (ESS)3000
- Basic knowledge of IBM Spectrum Scale
- Basic knowledge of DGX A100 systems
- Basic knowledge of NVIDIA switches
- Basic knowledge of InfiniBand Networking Technologies

Introduction

The adoption of GPU-accelerated computing infrastructure has become imperative to support deep learning (DL) and other computationally intensive workloads. GPUs enable working with large data sets and real-time streaming that is not possible on other platforms. However, accelerated computing needs to be matched with storage and networking that is also capable of large, diverse, and real-time data management.

The IBM Storage with NVIDIA DGX A100 systems reference architecture provides a prescriptive solution for IT administrators to deploy a validated solution with shared, extensible storage that is designed for DL, inference, data exploration, and other computationally and I/O-intensive work.

For the IT administrator, this reference architecture provides the specifications for networking, storage, and infrastructure that have been proven to enable improved scalability, performance, and cost-effective manageability.

For the data scientist, team productivity, data reuse, and logical data locality can be enhanced through shared storage that can integrate with and enhance the DL workflow.

Designed as a scalable unit that can be scaled to meet growing business and research needs, the IBM Storage with NVIDIA DGX A100 systems supports organizations looking to satisfy the needs for multiple workloads, from providing “as-a-Service” access for small interactive jobs, to supporting cluster-wide jobs that make the full use of multi-GPU and multi-node resources. IBM Storage provides a storage framework with scalability, extensibility, and the enterprise attributes required, including data protection, data tiering, and hybrid cloud integration.

The Artificial Intelligence Ladder

Data is the fuel for artificial intelligence (AI). The best AI is built on a foundation of data that is collected and organized as carefully as it is analyzed and then infused into the business. Organizations are challenged with gaining insights from their data for many reasons. Data silos make it difficult to get a holistic view of all your information, limiting the value of AI. Current infrastructure that was not built for AI is not flexible enough to respond to new demands without adding complexity.

Every successful AI project goes through a multi-step process (Figure 1) that starts with having the right data and progresses to using AI broadly.

Collect

Data is the fuel that powers AI, but it can become trapped or stored in a way that makes it difficult or cost prohibitive to maintain or expand. IBM Storage makes data simple and accessible for a hybrid cloud infrastructure.

Figure 1: The AI Ladder

Organize

AI can only be as good as the data it relies on. Businesses must fully understand what data they have so they can leverage it for AI and other organizational needs, including compliance, data optimization, data cataloging and data governance.

Analyze

Organizations must plan for opportunities beyond the development of AI; they need to build AI infrastructures with confidence in scalability, high performance, and extensibility to the data lake and the storage catalog.

Infuse

Business challenges can become an opportunity to explore, understand, predict, and bring an AI infrastructure to your entire organization. IBM Storage is empowering customers to use data and AI storage in order to leverage that infrastructure in more ways that bring value to the organization.

Solution Components

IBM Storage for Data and AI

IBM Storage for Data and AI covers the complete use case for Big Data and AI applications across hybrid cloud. The integrated approach provides a management framework and unified view of enterprise and research data across multiple data sources and applications. With the ability to support the entire AI ladder, IBM reduces costs and enables data scientists to rapidly identify and use relevant data. Highly flexible and extremely scalable, IBM Storage for Data and AI may be deployed on and integrate with multiple platforms and clouds.

There are three independent, yet integrated offerings in the software-defined portfolio.

- **IBM Spectrum Scale** provides scalable file storage, multi-protocol access, and data peering with IBM COS.
- **IBM Cloud Object Storage** (IBM COS) is an efficient and secure data lake for object applications or backing multiple services.
- **IBM Spectrum Discover** provides the data catalogue and custom data tagging across platforms.

IT and end-users can use a programmatic interface for data discovery, storage efficiency, and workflow optimization. IBM Storage for Data and AI provides multiple deployment options with IBM solutions, software-defined storage, or on public cloud providers such as IBM Cloud, AWS, Azure and Google.

IBM Spectrum Scale, IBM COS, and IBM Spectrum Discover provide the data scientist and the IT administrator performance, optimized data tiering, and data tracking that can reduce costs and improve productivity. Together, they represent the Storage for AI and Big Data part of the IBM storage portfolio that covers primary block storage with all-flash arrays, modern data protection, and software-defined storage. (Figure 2).

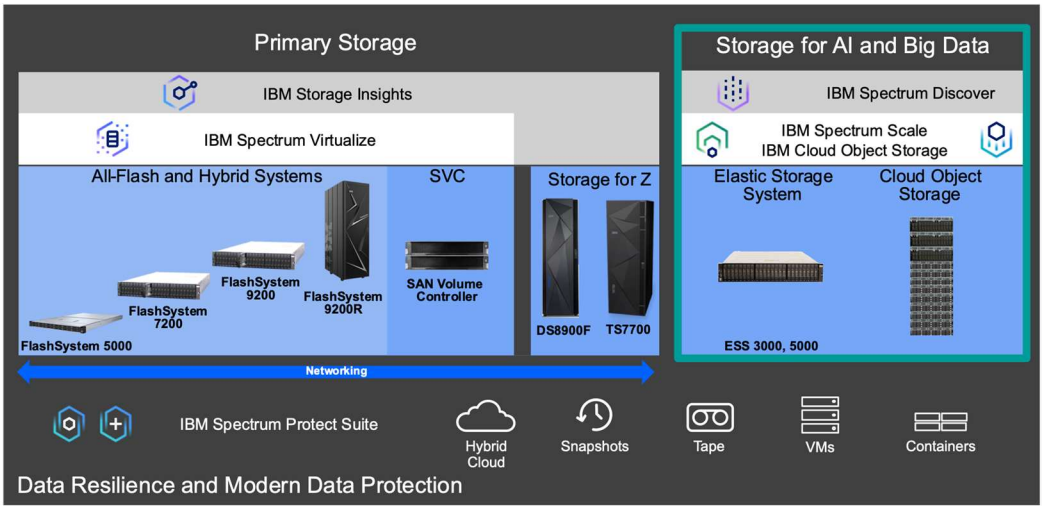

Figure 2: IBM Storage Portfolio

IBM Spectrum Scale

IBM Spectrum Scale is an industry leader in high-performance file systems. The underlying parallel filesystem provides scalable throughput and low latency data access, as well as superior metadata performance. Unlike NFS systems that can easily bottleneck, the distributed architecture of a parallel filesystem provides reliable performance for multi-user sequential and random read or write. IBM Spectrum 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 Spectrum Scale v5 has been optimized for modern AI workloads. Remarkably fast directory and file metadata management is required for the many AI/ML workloads that distribute data across multiple directories or many files.

With IBM Spectrum Scale, a DGX POD deployment may share data with existing infrastructure, such as an HPC cluster, Hadoop/Spark, or a structured data source. IBM Spectrum Scale creates a single namespace (or data plane) across systems. For users, it is a single repository that can access NFS, SMB, Object, or high-performance native POSIX filesystem. This single data plane allows the data administrator, analyst, or data scientist to access all the data in place. The entire data pipeline, from ingest to inference can be completed without having to make additional copies or move data between systems. Multiple clusters can be integrated into a single namespace to provide rapid local access to logically or geographically distributed data.

Although not in the scope of this Reference Architecture, an DGX POD may also be backed up by other storage. IBM Spectrum Scale enables data to be tiered automatically and transparently to and from more cost-effective storage, including hard disk drive (HDD), tape, and cloud. The software provides automated, policy driven, or workload directed data tiering to optimize performance and costs. When deployed with IBM Cloud Object Storage, or AWS S3, IBM Spectrum Scale has high-performance object tiering for transparent bi-directional data sharing. Data may be written or read as objects and still be available to be run on a DGX POD with IBM Spectrum Scale.

IBM Spectrum Scale provides Container Native Access and Operators to support Kubernetes driven DevOps and Data Ops practices. In addition, IBM Spectrum Scale provides enterprise features such as call-home proactive support, encryption, and audit file logging that works with Qradar and Splunk SEIM platforms.

IBM Elastic Storage System (ESS) 3000

The IBM Elastic Storage System 3000 (Figure 3) combines the performance of NVMe storage technologies with the reliability and the rich features of IBM Spectrum Scale, along with several high-speed attachment options such as 100 Gb/s Ethernet and InfiniBand (IB) — all in a powerful 2U storage system.

Figure 3: IBM Elastic Storage System 3000

IBM Spectrum Scale on NVMe is designed to be the market leader in all-flash performance, and scalability with a bandwidth of around 40 GB/s per NVMe all-flash appliance and 100 microseconds latency. Providing data-driven multicloud storage capacity, the NVMe all-flash appliance is deeply integrated with the software defined capabilities of IBM Storage for Data and AI to seamlessly plug it into an analytics, scalable cluster, or AI workload.

Available with multiple drive options and advanced erasure coding, the IBM ESS 3000 provides options to optimize costs for different installation sizes. As with all IBM Spectrum Scale solutions, capacity and performance can be scaled. Combining ESS 3000 systems provides nearly linear performance scalability. IBM ESS 3000 solutions may also be used as an all-flash NVMe performance tier on slower storage, including tape or object storage. Table 1 shows some key specifications of the IBM ESS 3000 system.

System Features	• Dual 2-socket Storage Controllers, Active/Active • 384 GB or 768 GB memory per controller • De-Clustered RAID supporting erasure coding schemas: 3-way replication, 4-wayreplication, 4+2P, 4+3P, 8+2P, 8+3P
Performance	• Sequential read performance up to 42G B/s • Sequential write performance up to 32 GB/s
Networking	• EDR IB, up to 12 ports• 100G Ethernet, up to 12 ports
Drive Support	12 or 24 NVMe SSDs (1.92 TB, 3.84 TB, 7.68 TB or 15.36 TB)

Table 1: IBM Elastic Storage System 3000 Specifications

For detailed ESS3000 specifications, please refer the link
https://www.ibm.com/us-en/marketplace/elastic-storage-system-3000

NVIDIA DGX A100 System

The DGX A100 system (Figure 4) is the universal system for all AI workloads, offering unprecedented compute density, performance, and flexibility in the world's first 5 peta FLOPS AI system. The DGX A100 system features the world's most advanced accelerator, the NVIDIA A100 Tensor Core GPU, enabling enterprises to consolidate training, inference, and analytics into a unified, easy-to-deploy AI infrastructure.

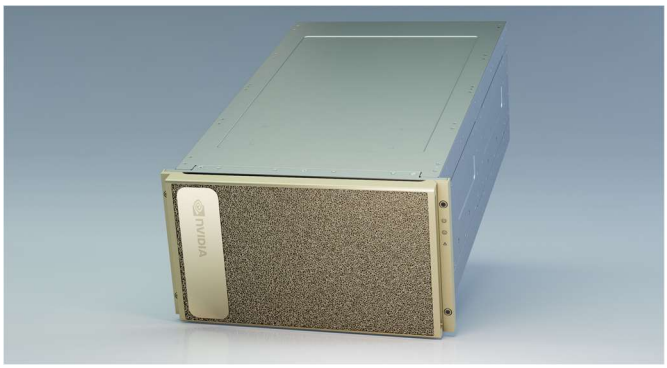

Figure 4: DGX A100 system

NVIDIA Mellanox Quantum QM8700 InfiniBand Switch

The InfiniBand converged fabric used for both compute and storage utilizes NVIDIA® Mellanox Quantum™ HDR 200 Gb/s InfiniBand Smart Switches (Figure 5).

Figure 5: NVIDIA Mellanox QM8700 HDR 200 Gb/s InfiniBand Switch

Each switch includes 40 QSFP56 ports, which are used for both communication to each DGX A100 system, as well as between switches in the compute fabric. All connections are HDR, maximizing the bandwidth between network elements. No InfiniBand partitions, or other segmentation is used, with the QM8700 switch providing the subnet manager for the compute fabric. Connection to the out-of-band management ports on the switch to the out-of-band management fabric may be done if needed, but is not critical to the operation of the DGX POD

NVIDIA NGC

The NVIDIA NGC™ (Figure 6) provides a range of options that meet the needs of data scientists, developers, and researchers with various levels of AI expertise. These users can quickly deploy AI frameworks with containers, get a head start with pre-trained models or model training scripts, and use domain specific workflows and Helm charts for the fastest AI implementations, giving them faster time-to-solution.

Spanning AI, data science, and HPC, the container registry on NGC features an extensive range of GPU-accelerated software for NVIDIA GPUs. The NGC hosts containers for the top AI and data science software. Containers are tuned, tested, and optimized by NVIDIA. Other containers for additional HPC applications and data analytics are fully tested and made available by NVIDIA as well. NGC containers provide powerful and easy-to-deploy software proven to deliver the fastest results, allowing users to build solutions from a tested framework, with complete control.

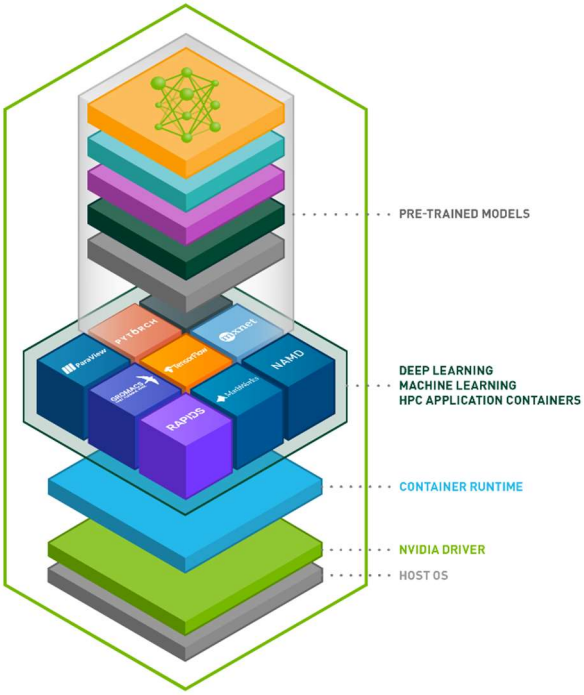

Figure 6: NGC Components

NGC offers step-by-step instructions and scripts for creating DL models, with sample performance and accuracy metrics to compare your results. These scripts provide expert guidance on building DL models for image classification, language translation, text-to-speech and more. Data scientists can quickly build performance-optimized models by easily adjusting hyperparameters. In addition, NGC offers pre-trained models for a variety of common AI tasks that are optimized for NVIDIA Tensor Core GPUs and can be easily re-trained by updating just a few layers, saving valuable time.

Solution Validation

This section describes the lab architecture, configuration, and validation of the NVIDIA DGX A100 systems with the IBM Spectrum Scale on IBM ESS3000 with QM8700 switches (Figure 7).

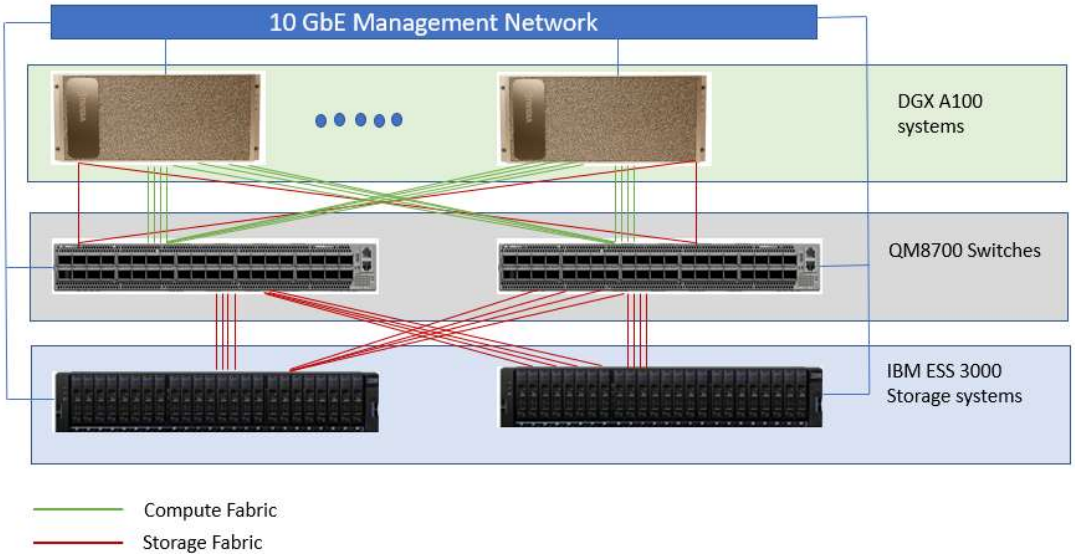

Figure 7: Converged Architecture for NVIDIA DGX A100 systems with IBM Storage

The converged infrastructure was created using QM8700 switches for both Compute fabric and Storage fabric to simplify network administration and deployment.

The DGX POD has Compute and Storage fabric networks:

- **Compute fabric.** Connects the eight 200 Gb NVIDIA Mellanox ConnectX®-6 HCAs from each DGX A100 system through separate network planes for inter-node communication. These adapters are configured in InfiniBand mode.
- **Storage fabric.** Connects two 200 Gb/s NVIDIA Mellanox ConnectX-6 HCAs from each DGX A100 system for storage communication purpose. This design document recommends InfiniBand for more throughput and network simplification.

LAB Testing

This section describes the various performances tests run on the IBM ESS3000 platform in the NVIDIA RAP Lab.

NVIDIA Collective Communications Library (NCCL) scalability test

Various tests are performed to validate the scalability of GPU to GPU communication across the multiple DGX A100 systems in the POD. Multi-node job scheduling requires high performance and low latency RDMA communication between the nodes in the DGX POD. Test results the show the scalable bandwidth between the NVIDIA DGX A100 systems required for multi-node DL workloads in Figure 8.

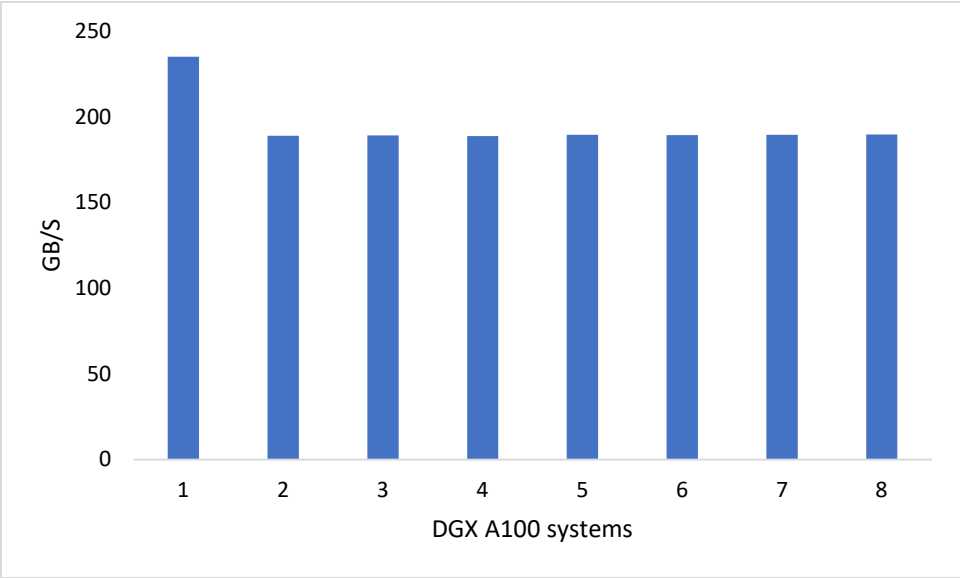

Figure 8: NCCL bandwidth performance for DGX A100 systems

Fio Bandwidth Test:

Flexible IO tester (FIO) is an open-source benchmark tool used for testing the storage bandwidth. FIO bandwidth tests were performed to measure the storage bandwidth from each DGX A100 system. Tests were simulated to run with both 100% reads and 100% writes with the below parameters

direct=1
ioengine=posixaio
iodepth=32
blocksize=1024k
size=4194304k
numjobs=120

The total system throughput performance for one to eight DGX A100 systems with the two IBM ESS 3000 units shows the performance scaling or reads (Figure 9) and writes (Figure 10) as systems are added. Two IBM ESS 3000s provide sufficient bandwidth to meet the throughput needs of eight DGX A 100 systems running the tested workloads. However, should additional throughput be needed for a different workload, a third IBM ESS 3000 can be easily added to the network and deliver additional throughput.

Figure 9 shows the total system read throughput scales to deliver of 94 GB/s with two ESS 300 units and eight DGX A100 systems.

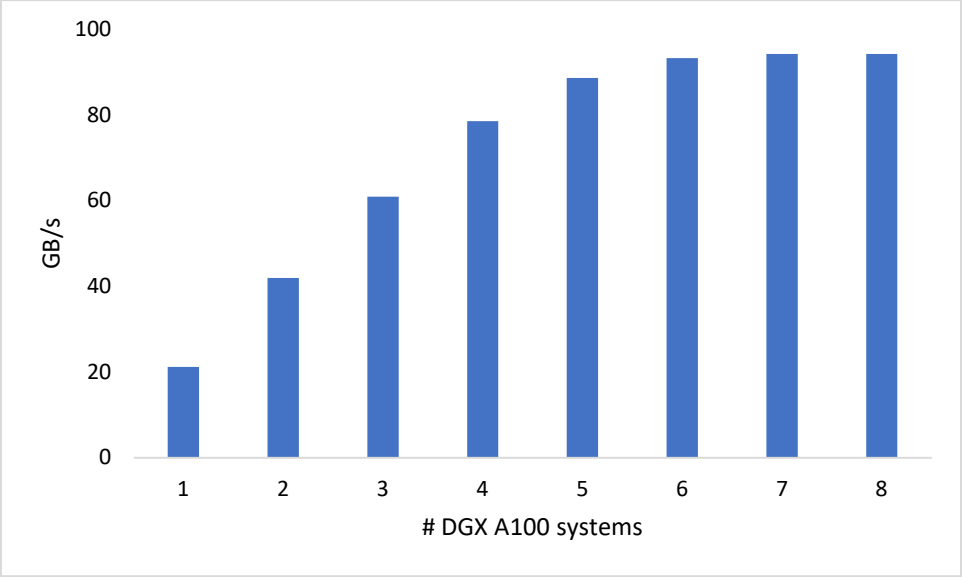

Figure 9: 8 node DGX A100 read performance with 2 x IBM ESS 3000 systems

Figure 10 shows the total system write throughput scales to 62 GB/s with two ESS units and eight DGX A100 systems.

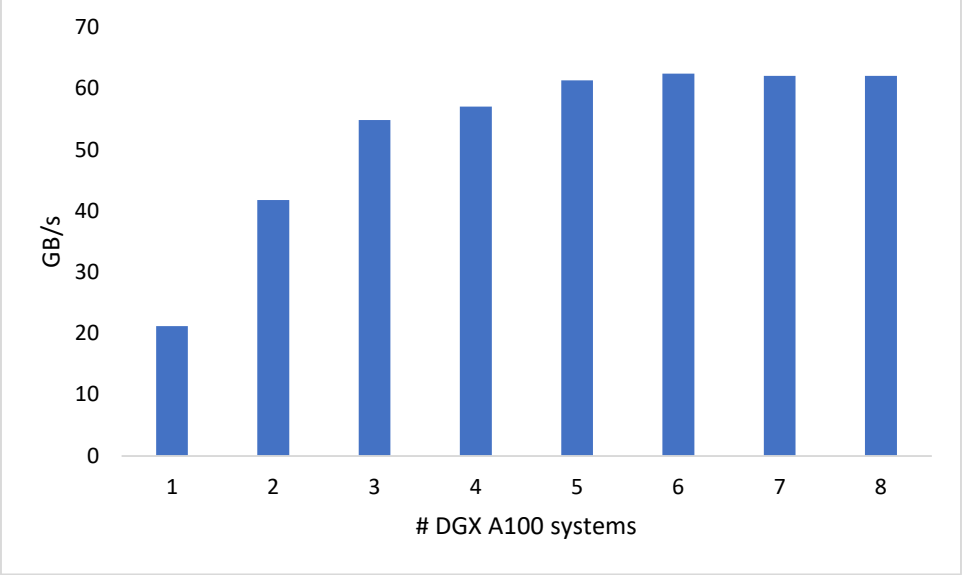

Figure 10: 8 node DGX A100 write performance with 2 x IBM ESS 3000 systems

IBM Spectrum Scale solutions scale almost linearly as storage systems are added. Results of the testing in Figure 11 demonstrates the read performance with the addition of a second IBM ESS 3000. Each IBM ESS 3000 delivers around 48 GB/Sec and scales almost linearly with the addition of an IBM ESS 3000 system to the same IBM Spectrum Scale storage instance.

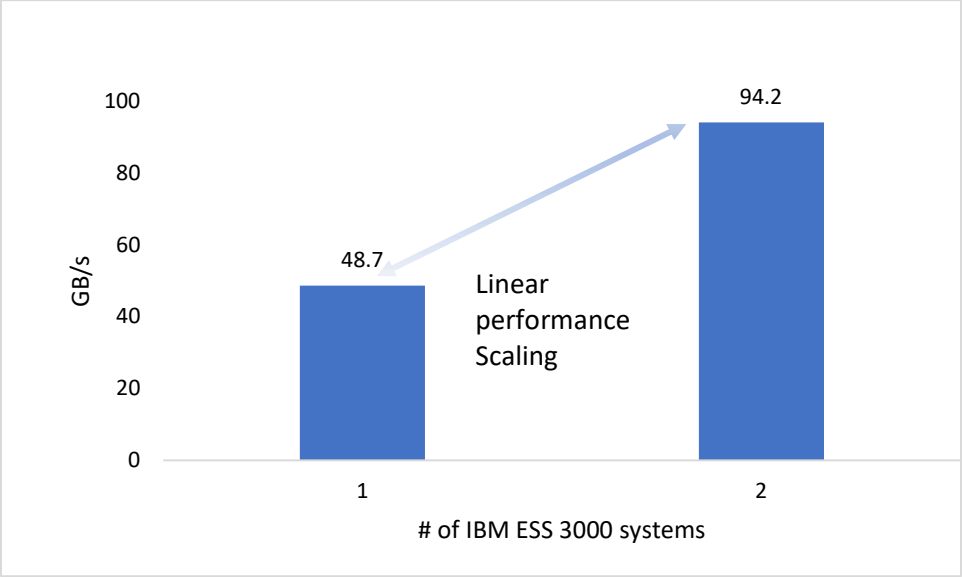

Figure 11: IBM ESS 3000 performance Scaling linearly

The results demonstrate that the ESS 3000 solution maximizes the potential throughput of the data infrastructure, scaling linearly from around 48 GB/s read performance for one ESS 3000 unit and also with two ESS 3000 units in only 4 units of rack space. Due to the composable scalability, extremely large, high-performance storage can be delivered using IBM ESS solutions with IBM Spectrum Scale.

MLPerf test

MLPerf is the industry standard set of benchmark implementations of neural networks and it measures how fast a system can perform training and inferencing of the DL models. Configurations were tested with one, two, four and eight DGX A100 systems and two IBM ESS 3000 systems to measure the operation of DL workloads.
This test used the MXNet implementation of ResNet-50 along with the ImageNet dataset.

The training results were measured at Epoch 0 and compared to the overall run average time for measuring the storage system read bandwidth during the validation. Epoch 0 is the most I/O intensive portion of the MLPerf benchmark run and time to insight is dependent on the Storage system performance.

IBM storage solutions demonstrate the linear scaling of the DGX POD with the additional DGX A100 systems added to the infrastructure. The results of the MLPerf performance in Figure 12 demonstrate the Multi-GPU scaling of the solution with the IBM Storage systems without data bottlenecks. It delivers linear scaling of time to insights as more DGX A100 systems are added to the DGX POD and reduces the time to insights to under 7 minutes with eight DGX A100 systems running with the two IBM ESS 3000 systems.

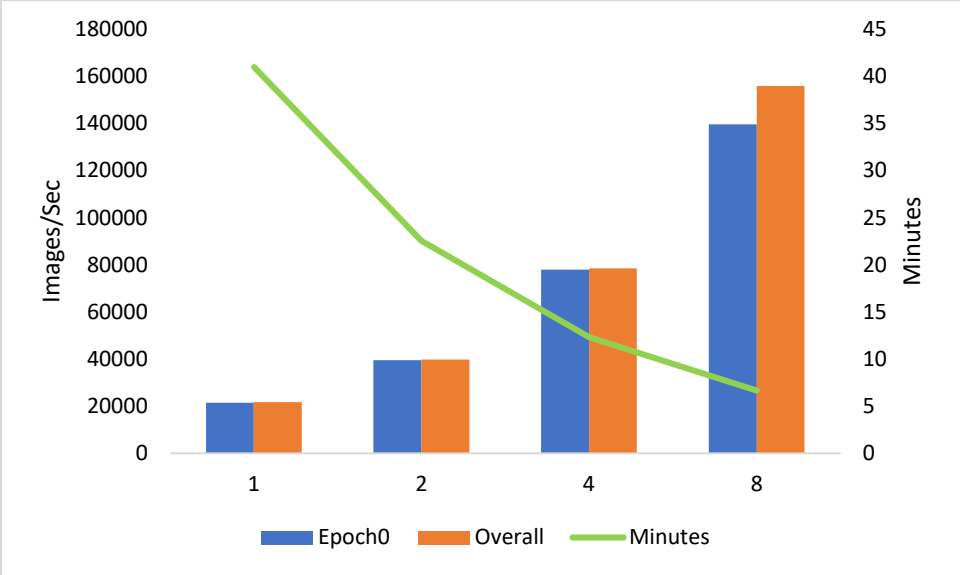

Figure 12: MLPerf ResNet-50 Performance

Solution Sizing Guidance

This reference architecture intends to provide the various configuration guidelines to the customers and partners planning to implement a DL infrastructure with the NVIDIA DGX A100 systems and IBM Storage systems. We focused on three rack configurations sized for different starting points (Figure 13). These are building blocks with which data and IT teams can growth from two to eight nodes. Though the deployment architecture is not in scope for this paper, the single name space of IBM Spectrum Scale also readily adapts to multi-rack scaling and larger clusters.

Figure 13: Two, four, and eight DGX A100 system configurations

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2:1 configuration
Two DGX A100 systems with one IBM ESS 3000 systems

Figure 14 depicts the two DGX A100 system configuration with the one IBM ESS 3000 systems using QM8700 IB switches. This configuration delivers up to 40 GB/s read performance from a single ESS 3000 system. Each DGX A100 system delivers 20 GB/s read performance using 200 Gb/S HDR connection configured for the storage usage.

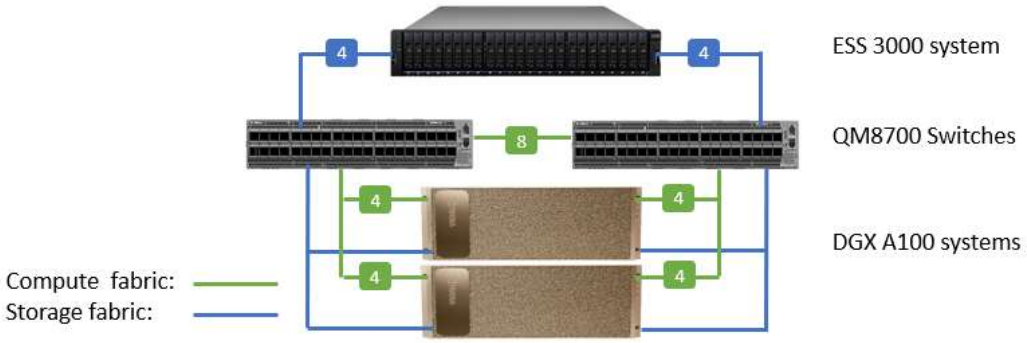

Figure 14: 2:1 configuration – Two DGX A100 systems with one IBM ESS 3000 system

4:1 configuration
Four DGX A100 systems with one IBM ESS 3000 systems

Figure 15 depicts the 4 DGX A100 system configuration with the one IBM ESS 3000 systems using QM8700 IB switches. This configuration delivers up to 48 GB/s read performance from a single ESS 3000 system, which is around 12 GB/s per DGX A100 system.

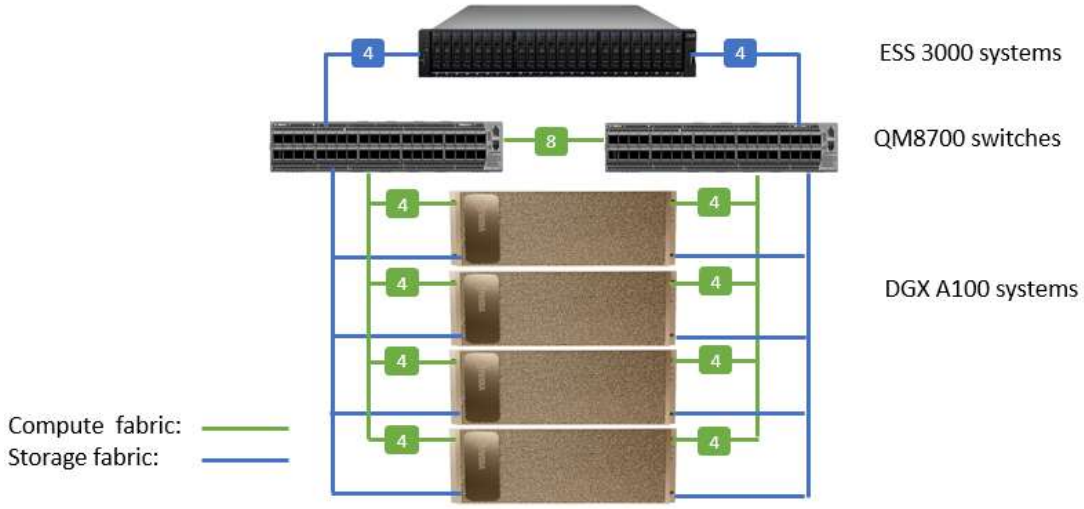

Figure 15: 4:1 configuration – Four DGX A100 systems with one IBM ESS 3000 system

8:2 configuration
8 DGX A100 systems with two IBM ESS 3000 systems

Figure 16 depicts the eight DGX A100 system configuration with two IBM ESS 3000 systems using QM8700 IB switches. This configuration delivers up to 94 GB/s read performance from a single GPFS file system configured using two IBM ESS systems. This configuration delivers more than 10 GB/s read performance per DGX A100 system.

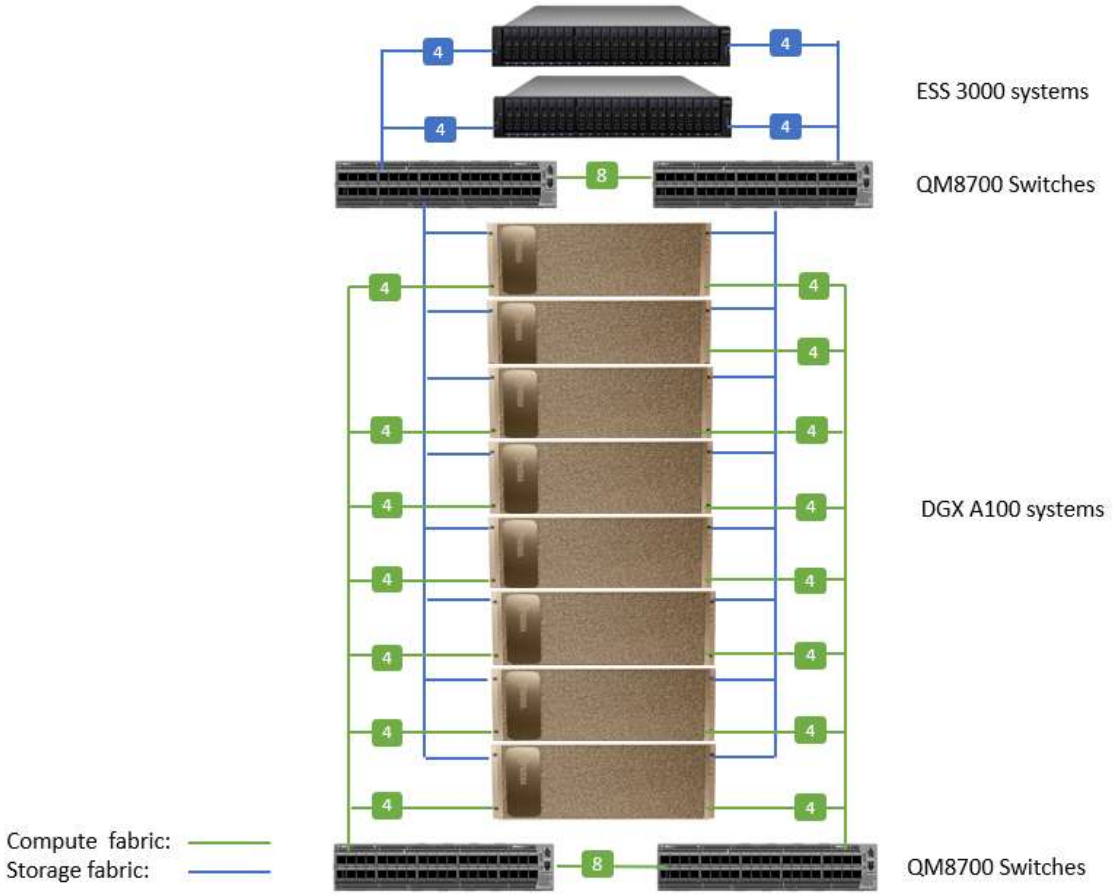

Figure 16: 8:2 configuration – Eight DGX A100 systems with two IBM ESS 3000 systems

Conclusion

The IBM Storage architecture over an NVIDIA IB fabric provides converged infrastructure for both compute and Storage fabric. IBM Storage provides a leading-edge performance for DL workload with high bandwidth and low latency for full utilization of GPUs when running on multiple DGX A100 systems as our tests have demonstrated.

IBM Storage for Data and AI and the NVIDIA DGX POD systems integrated with the NGC Software Stack provides the workload consolidation, data preparation and

management, and process automation that organizations seek to streamline end-to-end AI data pipeline development and ease integration into existing infrastructure

Get more Information

To learn more about the IBM, Mellanox, and SAS products and capabilities, contact your IBM representative or IBM Business Partner, or visit the following websites:

- IBM Spectrum Scale:
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  https://www.ibm.com/us-en/marketplace/elastic-storage-system-3000
- NVIDIA DGX A100 Systems
  https://www.nvidia.com/en-in/data-center/dgx-a100/

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