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Deployment Guide Cisco Public

# Scaling FlexPod for GPU Intensive Applications

# Model Simulations and Complex Data Analysis

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In partnership with:



## About the Cisco Validated Design Program

The Cisco Validated Design (CVD) program consists of systems and solutions designed, tested, and documented to facilitate faster, more reliable, and more predictable customer deployments. For more information, go to: <u>http://www.cisco.com/go/designzone</u>.

## **Executive Summary**

Organizations across various industries are facing challenges in overcoming competitive pressures, improve quality, boost productivity, accelerate digital transformation and decrease time to market, costs, and risks. The exponential growth in data is propelling the adoption of GPU Intensive Applications, HPC and AI technologies across multiple domains, as organizations seek to harness the power of these tools to extract meaningful insights, drive innovation, and make data-driven decisions in an increasingly data-rich world.

The definition of HPC (High-Performance Computing) is constantly changing, traditionally focused on transports that are sensitive to latency and the highest level of parallelization. GPUs take this evolution a step further. These advancements are enhanced by the amalgamation of GPU-accelerated applications and AI, leading to significant breakthroughs in various fields such as healthcare, finance, materials science, and climate research. This fusion allows researchers to delve into more complex models, simulate real-world scenarios, and analyze large datasets for data-driven discoveries. To fully leverage these capabilities and reap maximum benefits, a well-balanced and high-performing infrastructure encompassing compute, network, and storage is necessary. FlexPod facilitates this comprehensive approach.

Al has made a significant impact by transforming how the IT systems and services are developed, managed, and utilized. Adoption of Al-native infrastructure includes hardware accelerators such as GPU (Graphics Processing Unit), FPGA (Field Programmable Gate Arrays) and Tensor Processing Units (TPU) to handle Al computation effectively at scale. capable of extracting insights, learning from data patterns, and generating predictions, and making intelligent decisions, all at a scale and speed previously unattainable. Convergence of HPC and Al are reshaping the future datacenter design paradigm.

The convergence of GPU Intensive Applications, High-Performance Computing (HPC) and Artificial Intelligence (AI) technologies in a unified architecture brings about enhanced performance, scalability, and versatility for data-intensive tasks. This integration seamlessly incorporates popular AI development frameworks like TensorFlow and PyTorch, allowing data scientists and researchers to develop, train, and deploy AI models within the HPC environment. The fusion of custom solutions, hyperparameter optimization, and cross-validation enables the fine-tuning of models, empowering the exploration of complex scenarios and analysis of vast datasets in fields such as healthcare, finance, materials science, and climate research. Groundbreaking advancements are evident in applications like climate modeling, weather prediction, finance (risk analysis and fraud detection), energy exploration, material science, and healthcare (drug discovery and patient care).

While challenges exist, addressing them through strategic approaches involving talent development, best practices, robust data governance, and awareness of evolving technologies and regulations can unlock the transformative benefits of HPC and AI integration. This collaborative approach fosters improved decision-making, scientific advancements, and innovation across diverse industries and research domains.

This document summarizes <u>SpecHPC 2021</u> based benchmark applications targeted for real-life model simulation in the fields of but not limited to; linear scalability when executing various size of dataset on HPC cluster consisting of eight node Cisco UCS C240 M7 Rack Server hosting NVIDIA A100-80G GPUs in FlexPod architecture.

- Weather simulation Weather forecasting and climate modeling, agriculture, aviation, natural disaster prediction and prevention, renewable energy.
- Nuclear engineering (radiation transport) Nuclear energy, radiation shielding, nuclear security and safeguards, medical imaging, and treatment.
- High performance geometric multigrid Biomedical simulation, oil and gas reservoir simulation, Fluid Dynamics and Aerodynamics, structural mechanics.

FlexPod is designed to meet the demands of Al workloads. It offers:

- Simplified deployment and operation of general-purpose AI workloads.
- Seamless integration into AI eco systems.
- Gain operational simplicity and efficiency.
- Accelerate time to value and speed up AI implementation.
- Protect AI infra to safeguard systems, management, data, and applications.
- Linear Scalability: Demonstrated through benchmark tests, showcasing consistent performance even with varying dataset sizes.
- Centralized Management and Automation: Powered by Cisco Intersight, FlexPod reduces deployment times, optimizes resource utilization, minimizes energy consumption, and streamlines operations.
- NVIDIA HPC-X Software Toolkit Setup and Configuration: We've validated FlexPod using the NVIDIA HPC-X software toolkit, ensuring seamless integration and optimal performance. This toolkit harnesses the power of technologies like MPI (Message Passing Interface), OpenACC (Open Accelerators), and UCX (Unified Communication X) to enhance the capabilities of our solution.
- NetApp Tools: NetApp DataOps Toolkit is a Python library that makes it easy for developers, data scientists, and data engineers to perform numerous data management tasks.
- Comprehensive Testing for Real-World Workloads: Our rigorous testing process evaluates the scalability
  of FlexPod across different dataset sizes and application areas. We compare CPU-only performance with
  GPU-equipped systems, providing valuable insights into the capabilities of our solution.

The pre-validated design of FlexPod with centralized management and automation capabilities of Cisco Intersight reduces deployment times, optimize resource utilization, minimize energy consumption, and streamlining operations leading to better TCO (Total Cost of Ownership) and improved ROI (Return on Investment).

## Solution Overview

This chapter contains the following:

- <u>Audience</u>
- Purpose of this Document
- What's New in this Release?
- Solution Summary

The FlexPod AI (Artificial Intelligence) solution for HPC and AI workloads aims to deliver a seamless integration of the current FlexPod portfolio to enable single architecture which can be sized and optimized for GPU acceleration and faster access to data through high-speed data-fabric.

This document describes steps to install and configure the Cisco UCS C240 M7 Rack Server with NVIDIA GPU in FlexPod AI. The deployment details can be extended on the Cisco UCS server with supported NVIDIA GPUs such as Cisco UCS C22X M7, C24X M7 and Cisco UCS X210c compute nodes with X440p PCIe node within the FlexPod AI.

## Audience

The intended audience for this document includes, but is not limited to, sales engineers, field consultants, professional services, IT managers, IT engineers, partners, and customers who wants to take advantage of an infrastructure catering diverse workload HPC, AI/ML and analytics in a single architecture and be able to deliver IT efficiency and enable IT innovation.

## **Purpose of this Document**

This document serves as a comprehensive guide for integrating the Cisco Intersight-managed Cisco UCS M7 servers into the FlexPod AI infrastructure. It provides essential design guidance, covering various elements and considerations necessary for a successful deployment. This document highlights the significant value of horizontal scaling in accelerating applications through the addition of GPU and CPU resources. Horizontal scaling enables organizations to harness the power of multiple GPUs and CPUs, unlocking enhanced processing capabilities and improved performance for AI/ML workloads. By leveraging the scalability of the Cisco UCS M7 servers, businesses can achieve optimal utilization of computational resources and drive breakthroughs in fields that demand intensive computing power. Additionally, this document emphasizes the design and product requirements for incorporating scalable AI/ML solutions to address high-performance computing use cases, including weather modeling, high energy physics, scientific experiment simulation, and life sciences.

Furthermore, through the integration of Cisco Intersight management and the FlexPod AI infrastructure, this document provides valuable insights into the best practices and considerations for deploying a scalable and high-performing solution. It empowers organizations to leverage advanced technologies and accelerate their AI/ML initiatives, ultimately driving innovation and achieving transformative results in their respective industries.

## What's New in this Release?

The following design elements distinguish this version of FlexPod from previous models:

- Optimized integration of Cisco UCS C240 M7 servers with NVIDIA A100 GPU into the platform design.
- Scalable HPC cluster with GPU (Nvidia A100) and CPU (Intel 4<sup>th</sup> gen scalable processors) based practices.
- Support for 4<sup>th</sup> Gen Intel Xeon Scalable Processors (Sapphire Rapids) with up to 60 cores per processor and up to 8TB memory with 32 x 256GB DDR5-4800 DIMMs.

- Integration of NetApp A400 NVMe based all flash storage system to support AI/ML dataset.
- NetApp ONTAP 9.12.1.
- FlexPod Al architecture with end-to-end 100Gbps.
- Cisco Intersight managed stand-alone UCS C-Series rack server connected to Cisco Nexus switch.
- Cisco Intersight automated operating system installation.
- Ansible for post-OS configuration of HPC-AI cluster on bare metal.

## **Solution Summary**

The FlexPod AI solution offers the following key benefits:

- **Converged Infrastructure:** FlexPod provides a pre-validated and integrated solution that combines compute, storage, and networking components, streamlining deployment and management.
- **Modular Scalability:** With its modular architecture, FlexPod allows for the independent scaling of resources, enabling organizations to adapt to changing workload demands.
- **Simplified Management:** FlexPod includes management and orchestration tools that automate provisioning and ensure consistent and compliant infrastructure management.
- **Multitenancy Support:** It offers multitenancy capabilities, allowing multiple workloads or applications to run concurrently while maintaining isolation and security.
- **Compatibility Assurance:** Cisco and NetApp certification processes ensure that all components are compatible and reliable, reducing the risk of integration issues and providing stable and supported infrastructure.
- Investment protection: as technology evolves, businesses can add new components or upgrade existing
  ones to adapt to changing workload demands while maintaining the integrity of their initial investment in
  FlexPod.

## **Technology Overview**

This chapter contains the following:

- <u>FlexPod Al</u>
- <u>Cisco Unified Computing System</u>
- <u>Cisco UCS C-Series Rack Server</u>
- <u>Cisco Nexus 93600CD-GX</u>
- <u>NetApp AFF A-Series Storage</u>

## **FlexPod Al**

FlexPod is an integrated data center solution that combines compute, storage, and networking components, simplifying deployment, and offering scalability. It ensures compatibility and supports multiple workloads, making it an efficient and adaptable choice for modern data centers.

#### Figure 1. FlexPod AI components

## Networking

Cisco UCS Nexus 9000 series switch

Cisco UCS 6500 series Fabric Interconnect

## Compute

Cisco UCS X Series 9508 chassis with X210c M7 compute node and X440p PCIe node

Cisco UCS C Series Rack Server

## Storage

NetApp AFF A-Series All-Flash Storage Arrays







Go to the Cisco Design Zone for pre-validated <u>FlexPod Design Guides</u> containing a wide variety of enterprise applications.

## **Cisco Unified Computing System**

Cisco Unified Computing System (Cisco UCS) is a next-generation data center platform that integrates compute, network, storage, and virtualization resources into a single cohesive architecture simplifying data center management, improved operational efficiency, reduce total cost of ownership, and increase business agility.

Cisco UCS Manager is the central management software that provides a unified interface for configuring, monitoring, and automating the entire UCS infrastructure, streamlining operations and enabling rapid resource provisioning. Cisco Intersight is a cloud-based management platform that offers enhanced visibility, analytics, and automation for Cisco UCS and other Cisco infrastructure, providing a scalable and intelligent solution for optimizing data center operations and achieving agility in the modern IT landscape.

#### **Cisco UCS Differentiators**

Cisco Unified Computing System is revolutionizing the way servers are managed in the datacenter. The following are the unique differentiators of Cisco Unified Computing System and Cisco UCS Manager:

- Embedded Management–In Cisco UCS, the servers are managed by the embedded firmware in the Fabric Inter-connects, eliminating the need for any external physical or virtual devices to manage the servers.
- Unified Fabric-In Cisco UCS, from blade server chassis or rack servers to FI, there is a single Ethernet cable used for LAN, SAN, and management traffic. This converged I/O results in reduced cables, SFPs and adapters - reducing capital and operational expenses of the overall solution.
- Auto Discovery–By simply inserting the blade server in the chassis or connecting the rack server to the fabric interconnect, discovery and inventory of compute resources occurs automatically without any management intervention. The combination of unified fabric and auto-discovery enables the wire-once architecture of Cisco UCS, where compute capability of Cisco UCS can be extended easily while keeping the existing external connectivity to LAN, SAN, and management networks.

#### **Cisco Intersight**

Cisco Intersight is a lifecycle management platform for your infrastructure, regardless of where it resides. In your enterprise data center, at the edge, in remote and branch offices, at retail and industrial sites—all these locations present unique management challenges and have typically required separate tools. Cisco Intersight Software as a Service (SaaS) unifies and simplifies your experience of the Cisco Unified Computing System (Cisco UCS). See Figure 2.

#### Figure 2. Cisco Intersight



## **Cisco UCS C-Series Rack Server**

Cisco UCS C-Series Rack-Mount Servers keep pace with Intel Xeon and AMD EPYC processor innovation by offering the latest processors with increased processor frequency and improved security and availability features. Cisco UCS C-Series servers offer an improved price-to-performance ratio. They also extend Cisco UCS innovations to an industry-standard rack-mount form factor, including a standards-based unified network fabric, Cisco VN-Link virtualization support, and Cisco Extended Memory Technology.

It is designed to operate both in standalone environments and as part of Cisco UCS managed by <u>Cisco</u> <u>Intersight</u> or <u>Cisco UCS Manager</u>. Cisco UCS C-Series servers enable organizations to deploy systems incrementally–using as many or as few servers as needed–on a schedule that best meets the organization's timing and budget.

#### Cisco UCS C240 M7 Rack Server

The Cisco UCS C240 M7 Rack Server extends the capabilities of the Cisco UCS rack server portfolio with up to two 4th Gen Intel Xeon Scalable CPUs, with up to 60 cores per socket. The maximum memory capacity for 2 CPUs is 8 TB (for 32 x 256 GB DDR5 4800 MT/s DIMMs). The Cisco UCS C240 M7 has a 2-Rack-Unit (RU) form and supports up to 8 PCIe 4.0 slots or up to 4 PCIe 5.0 slots plus a modular LAN on motherboard (mLOM) slot. Up to five GPUs are supported. The server delivers significant performance and efficiency gains that will improve your application performance.

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Figure 3. Cisco UCS C240 M7 Rack Server - front and rear image

For more details, go to: Cisco UCS C240 M7 Rack Server Data Sheet.

## Cisco Nexus 93600CD-GX

Based on <u>Cisco Cloud Scale technology</u>, the Cisco Nexus 9300-GX switches are the next generation of fixed Cisco Nexus 9000 Series Switches capable of supporting 400 Gigabit Ethernet (GE). With the increase in use cases for applications requiring Artificial Intelligence (AI) and Machine Learning (ML), the platform addresses the need for high-performance, power-efficient, compact switches in the networking infrastructure. These switches are designed to support 100G and 400G fabrics for mobile service provider environments, including the network edge, 5G, IoT, Professional Media Networking platform (PMN), and Network Functions Virtualization (NFV).

The Cisco Nexus 93600CD-GX Switch (Figure 2) is a 1RU switch that supports 12 Tbps of bandwidth and 4.0 bpps across 28 fixed 40/100G QSFP-28 ports and 8 fixed 10/25/40/50/100/200/400G QSFP-DD ports.

Cisco provides two modes of operation for Cisco Nexus 9000 Series Switches. Organizations can deploy Cisco Application Centric Infrastructure (Cisco ACI) or Cisco NX-OS mode.

#### Figure 4. Cisco UCS Nexus 93600CD-GX Switch



For more details, see <u>https://www.cisco.com/c/en/us/products/collateral/switches/nexus-9000-series-</u> switches/nexus-9300-gx-series-switches-ds.html

## NetApp AFF A-Series Storage

NetApp AFF A-Series controller lineup provides industry leading performance while continuing to provide a full suite of enterprise-grade data management and data protection features. NetApp AFF A-Series systems support end-to-end NVMe technologies, from NVMe-attached SSDs to frontend NVMe over Fibre Channel (NVMe/FC) host connectivity. These systems deliver enterprise class performance, making them a superior choice for driving the most demanding workloads and applications. With a simple software upgrade to the modern NVMe/FC SAN infrastructure, you can drive more workloads with faster response times, without disruption or data migration. Additionally, more organizations are adopting a "cloud first" strategy, driving the need for enterprise-grade data services for a shared environment across on-premises data centers and the cloud. As a result, modern all-flash arrays must provide robust data services, integrated data protection, seamless scalability, and new levels of performance – plus deep application and cloud integration. These new workloads demand performance that first-generation flash systems cannot deliver.

For more information about the NetApp AFF A-series controllers, see the AFF product page: <u>https://www.netapp.com/us/products/storage-systems/all-flash-array/aff-a-series.aspx</u>.

You can view or download more technical specifications of the NetApp AFF A-series controllers here: <u>https://www.netapp.com/us/media/ds-3582.pdf</u>

#### NetApp AFF A400

The NetApp AFF A400 offers full end-to-end NVMe support. The frontend NVMe/FC connectivity makes it possible to achieve optimal performance from an all-flash array for workloads that include artificial intelligence, machine learning, and real-time analytics as well as business-critical databases. On the back end, the A400 supports both serial-attached SCSI (SAS) and NVMe-attached SSDs, offering the versatility for current customers to move up from their legacy A-Series systems and satisfying the increasing interest that all customers have in NVMe-based storage.

The NetApp AFF A400 offers greater port availability, network connectivity, and expandability. The NetApp AFF A400 has 10 PCIe Gen3 slots per high availability pair. The NetApp AFF A400 offers 25GbE or 100GbE, as well as 32Gb/FC and NVMe/FC network connectivity. This model was created to keep up with changing business needs and performance and workload requirements by merging the latest technology for data acceleration and ultra-low latency in an end-to-end NVMe storage system.



#### Figure 5. NetApp AFF A400 Storage - front and rear image

## NetApp ONTAP 9

NetApp storage systems harness the power of ONTAP to simplify the data infrastructure from edge, core, and cloud with a common set of data services and 99.9999 percent availability. NetApp ONTAP 9 data management software from NetApp enables customers to modernize their infrastructure and transition to a cloud-ready data center. ONTAP 9 has a host of features to simplify deployment and data management, accelerate and protect critical data, and make infrastructure future-ready across hybrid-cloud architectures.

NetApp ONTAP 9 is the data management software that is used with the NetApp AFF A400 all-flash storage system in this solution design. ONTAP software offers secure unified storage for applications that read and write

data over block- or file-access protocol storage configurations. These storage configurations range from highspeed flash to lower-priced spinning media or cloud-based object storage. ONTAP implementations can run on NetApp engineered FAS or AFF series arrays and in private, public, or hybrid clouds (NetApp Private Storage and NetApp Cloud Volumes ONTAP). Specialized implementations offer best-in-class converged infrastructure, featured here as part of the FlexPod AI solution or with access to third-party storage arrays (NetApp FlexArray virtualization). Together these implementations form the basic framework of the NetApp Data Fabric, with a common software-defined approach to data management, and fast efficient replication across systems. FlexPod and ONTAP architectures can serve as the foundation for both hybrid cloud and private cloud designs.

Read more about all the capabilities of ONTAP data management software here: <a href="https://www.netapp.com/us/products/data-management-software/ontap.aspx">https://www.netapp.com/us/products/data-management-software/ontap.aspx</a>

ONTAP 9.12 brings additional enhancements in manageability, data protection, networking and security protocols, and SAN and object storage. It also includes updated hardware support, increased MetroCluster IP solution scale, and supports IP-routed MetroCluster IP backend connections. See the ONTAP 9.12.1 release note below for more details: <u>https://docs.netapp.com/us-en/cloud-volumes-ontap-9121-relnotes/</u>

#### **FlexClone**

NetApp FlexClone technology enables instantaneous point-in-time copies of a FlexVol volume without consuming any additional storage until the cloned data changes from the original. FlexClone volumes add extra agility and efficiency to storage operations. They take only a few seconds to create and do not interrupt access to the parent FlexVol volume. FlexClone volumes use space efficiently, applying the ONTAP architecture to store only data that changes between the parent and clone. FlexClone volumes are suitable for testing or development environments, or any environment where progress is made by locking-in incremental improvements. FlexClone volumes also benefit any business process where you must distribute data in a changeable form without endangering the integrity of the original.

#### NetApp DataOps Toolkit

The NetApp DataOps Toolkit is a Python library that makes it easy for developers, data scientists, and data engineers to perform numerous data management tasks. These tasks include provisioning a new data volume or development workspace, cloning a data volume or development workspace almost instantaneously, and creating a NetApp Snapshot copy of a data volume or development workspace for traceability and baselining. This Python library can function as either a command-line utility or a library of functions that can be imported into any Python program or Jupyter Notebook.

The DataOps Toolkit supports Linux and macOS hosts. The toolkit must be used in conjunction with a NetApp data storage system or service. It simplifies various data management tasks that are executed by the data storage system or service. To facilitate this simplification, the toolkit communicates with the data storage system or service through an API.

The NetApp DataOps Toolkit for Kubernetes abstracts storage resources and Kubernetes workloads up to the data-science workspace level. These capabilities are packaged in a simple, easy-to-use interface that is designed for data scientists and data engineers. Using the familiar form of a Python program, the Toolkit enables data scientists and engineers to provision and destroy JupyterLab workspaces in just seconds. These workspaces can contain terabytes, or even petabytes, of storage capacity, enabling data scientists to store all their training datasets directly in their project workspaces. Gone are the days of separately managing workspaces and data volumes.

#### Figure 6. NetApp Data Science Toolkit



#### AI/ML Use Cases - DataOps for Data Scientist

With the NetApp DataOps Toolkit, a data scientist can almost instantaneously create a space-efficient data volume that's an exact copy of an existing volume regardless of the size of the dataset. Data scientists can quickly create clones of datasets that they can reformat, normalize, and manipulate, while preserving the original "gold-source" dataset. Under the hood, these operations use highly efficient and battle-tested NetApp FlexClone feature, but they can be performed by a data scientist without storage expertise. What used to take days or weeks (and the assistance of a storage administrator) now takes seconds.



Data scientists can also save a space-efficient, read-only copy of an existing data volume. Based on the famed NetApp Snapshot technology, this functionality can be used to version datasets and implement dataset-to-model traceability. In regulated industries, traceability is a baseline requirement, and implementing it is extremely complicated with most other tools. With the NetApp DataOps Toolkit, it's quick and easy.

More operations and capabilities are available and documented here: <u>https://github.com/NetApp/netapp-data-</u> science-toolkit

## Solution Design

This chapter contains the following:

- <u>Requirements</u>
- <u>Considerations</u>

## **Requirements**

The FlexPod AI with Cisco UCS and NetApp storage meets the following general design requirements:

- Resilient design across all layers of the infrastructure with no single point of failure.
- Scalable design with the flexibility to add compute capacity, storage, or network bandwidth as needed.
- Modular design that can be replicated to expand and grow as the needs of the business grow.
- Flexible design that can support different models of various components with ease.
- Simplified design with ability to integrate and automate with external automation tools.
- Cloud-enabled design which can be configured, managed, and orchestrated from the cloud using GUI or APIs.

To deliver a solution which meets all these design requirements, various solution components are connected and configured as explained in the following sections.

#### **Physical Components**

Table 1 lists the required physical components and hardware for FlexPod AI.

#### Table 1. FlexPod Al Hardware Components

Component	Hardware
Servers	Eight (8) Cisco UCS C240 M7 rack server
Storage	NetApp AFF A400
Network	Two (2) Cisco Nexus 93600CD-GX

#### Table 2. Cisco UCS C240 M7 Hardware Components

Component	Hardware		
Processor	Two (2) 4th Gen Intel® Xeon® Scalable Processor 6454S 32C/2.2GHz/270W		
Memory	Sixteen (16) 64GB DDR5-4800 RDIMM		
NIC (Network Interface Card)	Mellanox ConnectX-6 DX 2 x 100Gb Ethernet		
GPU (Graphics Processing Unit)	NVIDIA Tesla A100-80GB GPU		

#### Table 3. NetApp AFF A400 Components

Component	Hardware
AFF Flash Array	NetApp All Flash AFF A400 Storage Array (4RU)

Component	Hardware
Capacity	27.8TB (12 x 3.49TB NVMe SSD Drives)
Connectivity	4 x 100Gb/s (2 x 100Gb per controller) Data Rate: 100 Gb/s Ethernet, PCI Express Gen3: SERDES @ 8.0GT/s, 16 lanes) (MCX516A-CCAT) 1 Gb/s redundant Ethernet (Management port)

#### **Software Components**

<u>Table 4</u> lists the software components and the versions required for FlexPod AI as tested and validated in this document.

Component	Software version
Cisco Intersight	SaaS platform
Cisco UCS Server Firmware	4.3(2.230207)
Host OS	Ubuntu 22.04 LTS
Mellanox ConnectX-6 NIC	22.36.1010
	MLNX OFED 5.8-1.1.2.1
NVIDIA Tesla A100-80GB GPU	NVIDIA CUDA 12.2.2
	NVIDIA Driver 535.104.05
NetApp AFF A400	ONTAP 9.12.1
Cisco Nexus 93600CD-GX	NX-OS 10.3.3

Note: See the <u>Bill of Materials</u> section for a complete list and corresponding PID.

#### **Required VLANs**

<u>Table 5</u> lists various VLANs configured for setting up the FlexPod environment including their specific usage.

VLAN ID	Name	Usage
2	Native-VLAN	Use VLAN 2 as Native VLAN instead of default VLAN (1)
248	OOB-MGMT-VLAN	Management VLAN to access and manage the servers
110	AI-ML-NFS_1	NFS VLAN to access AI/ML NFS volume hosting HPC data
160	AI-ML-NFS_2	NFS VLAN to access AI/ML NFS volume hosting HPC data

 Table 5.
 FlexPod AI - VLAN Usage

Some of the key highlights of VLAN usage are as follows:

- Bare-metal servers are managed using same management in-band VLAN: IB-MGMT-VLAN (248).
- Utilizing dedicated NFS VLANs for HPC and AI; hosts provide path selection flexibility and the ability to configure specific QoS policies. You are encouraged to use separate, dedicated VLANs for NFS traffic.

#### **Physical Topology**





For this solution, we tested left side configuration as shown in <u>Figure 8</u> with Cisco UCS C-Series Rack Server and NetApp AFF A400 storage array connected to Cisco Nexus 93600CD-GX leaf switch with layer 2 configuration for a single rack testing. For large cluster spanning across multiple racks and Spine/Leaf networking best practices, please refer to <u>Cisco Data Center Networking Blueprint for AI/ML Applications</u>.

Note: This solution is tested with Cisco VIC 15428 (4x 10/25/50G mLOM C-Series) for 10GbE connection with ToR switch and utilized for separate OS management from data traffic on Mellanox ConnectX6-DX Ethernet NIC.

## **Logical Topology**

The single rack topology of the FlexPod AI architecture highlighted in this CVD can be easily expanded to a larger size cluster connecting hundreds of servers with Spine-Leaf network design where congestion management enabled on leaf layer and spine later with PFC and ECN as shown in Figure 9.



## Considerations

The information in this section is provided as a reference for cabling the physical equipment in a FlexPod environment. To simplify cabling requirements, a cabling diagram was used.

The cabling diagram in this section contains the details for the prescribed and supported configuration of the NetApp AFF 400 running NetApp ONTAP 9.12.1.

#### Tech tip

For any modifications of this prescribed architecture, consult the NetApp Interoperability Matrix Tool (IMT).

This document assumes that out-of-band management ports are plugged into an existing management infrastructure at the deployment site. These interfaces will be used in various configuration steps.

Be sure to use the cabling directions in this section as a guide.

The NetApp storage controller and disk shelves should be connected according to best practices for the specific storage controller and disk shelves. For disk shelf cabling, refer to <u>NetApp Support</u>.

Figure 10 details the cable connections used in the validation lab for the FlexPod topology based on the Cisco UCS C240 M7 stand-alone server managed via Intersight and NetApp AFF A400 storage array. Two 100Gb uplinks connect as port-channels from each Cisco UCS Nexus 93600CD-GX switches to the NetApp AFF controllers. Additional 1Gb management connections will be needed for an out-of-band network switch that sits apart from the FlexPod infrastructure. Each Cisco UCS C240 M7 rack server and Cisco Nexus switch is connected to the out-of-band network switch, and each AFF controller has a connection to the out-of-band

network switch. Layer 3 network connectivity is required between the Out-of-Band (OOB) and In-Band (IB) Management Subnets.



Figure 10. Physical cabling for Cisco UCS C-Series

## Install and Configure

This chapter contains the following:

- <u>Network Switch Configuration</u>
- <u>NetApp ONTAP Storage Configuration</u>
- Install Cisco UCS
- <u>Cisco Intersight Configuration</u>
- Post-OS Configuration
- Mellanox ConnectX-6 NIC Best Practice
- NVIDIA GPU Configuration for HPC Workload

## **Network Switch Configuration**

Designing a network infrastructure for an HPC and AI cluster requires careful consideration to ensure efficient data transfer, low latency, and scalability. The network configuration tuned to match the specific requirements of your HPC and AI workloads via implementation of QoS (Quality of Service) to ensure efficient utilization and monitoring of the network resources available.

Please refer to <u>Cisco Data Center Networking Blueprint for AI/ML Applications</u> for more detailed documentation on best practices for lossless network design and configuration required for HPC and AI workload.

This section provides a detailed procedure for configuring the Cisco Nexus 93600CD-GX switches for use in a FlexPod AI/ML environment. The Cisco Nexus 93600CD-GX will be used for LAN switching in this solution. This configuration allows deployment of Cisco AI/ML platforms in bare-metal server configuration.

#### **Tech tip**

The following procedures describe how to configure the Cisco Nexus switches for use in a base FlexPod environment. This procedure assumes the use of Cisco Nexus 9000 NX-OS 10.3.3F.

The following procedure includes the setup of NTP distribution on both the mgmt0 port and the in-band management VLAN. The interface-vlan feature and ntp commands are used to set this up. This procedure also assumes that the default VRF is used to route the in-band management VLAN.

This procedure sets up and uplink virtual port channel (vPC) with the IB-MGMT and OOB-MGMT VLANs allowed.

This validation assumes that both switches have been reset to factory defaults by using the "write erase" command followed by the "reload" command.

#### **Physical Connectivity**

Follow the physical connectivity guidelines for FlexPod as explained in the Physical Topology section.

#### **Initial Configuration**

The following procedures describe this basic configuration of the Cisco Nexus switches for use in the FlexPod environment. This procedure assumes the use of Cisco Nexus 9000 10.2(5)M, the Cisco suggested Nexus switch release at the time of this validation.

#### **Procedure 1.** Set Up Initial Configuration from a serial console

Step 1. Set up the initial configuration for the Cisco Nexus 93600CD-GX switch.

#### Procedure 2. Configure Global Settings on both Cisco Nexus Switches

#### Tech tip

Remote Direct Memory Access (RDMA) over Converged Ethernet (RoCE); for RoCEv2 transport, the network must provide high throughput and low latency while avoiding traffic drops in situations where congestion occurs.

The following procedures describe how to configure the Cisco Nexus switches global configuration highlighting for RoCE V2 and QoS, no-drop shown. Please refer Appendix for full configuration.

**Step 1.** Login as admin user into the Cisco Nexus switch A and run the following commands to set the global configuration on switch:

configure terminal

policy-map type network-qos qos\_network

class type network-qos c-8q-nq3

mtu 9216

pause pfc-cos 3

class type network-qos c-8q-nq-default

mtu 9216

class-map type qos match-any CNP

match dscp 48

class-map type qos match-all ROCEv2

match dscp 24,26

policy-map type qos QOS\_MARKING

class ROCEv2

set qos-group 3

class CNP

set qos-group 7

class class-default

set qos-group 0

policy-map type queuing QOS\_EGRESS\_PORT

class type queuing c-out-8q-q6

bandwidth remaining percent 0

class type queuing c-out-8q-q5

bandwidth remaining percent 0

class type queuing c-out-8q-q4

bandwidth remaining percent 0

class type queuing c-out-8q-q3

bandwidth remaining percent 50

random-detect minimum-threshold 150 kbytes maximum-threshold 3000 kbytes drop-probability 7 weight 0 ecn

class type queuing c-out-8q-q2

bandwidth remaining percent 0

class type queuing c-out-8q-q1

bandwidth remaining percent 0

class type queuing c-out-8q-q-default

bandwidth remaining percent 50

class type queuing c-out-8q-q7

priority level 1

system qos

service-policy type network-qos qos\_network

service-policy type queuing output QOS\_EGRESS\_PORT

copy running-config startup-config

**Step 2.** Login as admin user into Cisco Nexus Switch B; repeat steps 1 and 2 above to set up the global configuration.

#### Tech tip

Make sure to run copy run start to save the configuration on each switch after the configuration is completed.

## **NetApp ONTAP Storage Configuration**

#### NetApp AFF A-Series Storage System

NetApp AFF A-Series is a family of all-flash storage systems by NetApp. The systems are designed to provide high-performance, low-latency and highly available storage solution suitable for a wide range of enterprise applications such as AI/ML, databases, and virtualization.

NetApp storage systems support a wide variety of disk shelves and disk drives. The complete list of <u>disk</u> <u>shelves</u> that are supported by the AFF A400 is available at the <u>NetApp Support</u> site.

Follow the physical installation procedures for the controllers found here: <u>https://docs.netapp.com/us-</u> en/ontap-systems/index.html.

When using SAS disk shelves with NetApp storage controllers, refer to: <u>https://docs.netapp.com/us-en/ontap-system.html</u> for proper cabling guidelines.

When using NVMe drive shelves with NetApp storage controllers, refer to: <u>https://docs.netapp.com/us-en/ontap-systems/ns224/hot-add-shelf.html</u> for installation and servicing guidelines.

For more information about the setup and configuration of the NetApp AFF A-Series storage system setup and deployment FlexPod solution, go to:

https://www.cisco.com/c/en/us/solutions/design-zone/data-center-design-guides/flexpod-designguides.html

https://www.netapp.com/data-storage/flexpod/validated-designs/

## Install Cisco UCS

This section contains the following:

#### <u>Physical Connectivity</u>

#### Tech tip

Please visit Cisco UCS C240 M7 Server Installation and Service Guide: https://www.cisco.com/c/en/us/td/docs/unified\_computing/ucs/c/hw/C240M7/install/b-cisco-c240-m7-install/m-installing.html

Please visit GPU card installation on C240 M7:

https://www.cisco.com/c/en/us/td/docs/unified\_computing/ucs/c/hw/C240M7/install/b-cisco-c240-m7-install/m-gpuinstall.html

Please visit Cisco UCS C-Series Integrated Management Controller GUI Configuration Guide: https://www.cisco.com/c/en/us/td/docs/unified computing/ucs/c/sw/gui/config/guide/4 3/b cisco ucs c-series gui configuration guide 43.html

#### **Physical Connectivity**

To manage Cisco UCS C240 M7 Rack Server connected to Cisco Nexus switch directly; connect and configure Cisco Integrated Management Controller connect CIMC port to ToR (top of rack) switch as shown in <u>Figure 11</u>.

#### **Tech tip**

The Cisco IMC management service is used only when the server is operating in Standalone Mode. If your C-Series server is integrated into a UCS system, you must manage it using a Cisco UCS Fabric Interconnect running in either CSM or IMM. For information about using UCS Manager, see the configuration guides listed in the Cisco UCS B-Series Servers Documentation Roadmap at <a href="http://www.cisco.com/go/unifiedcomputing/b-series-doc">http://www.cisco.com/go/unifiedcomputing/b-series-doc</a>.

Figure 11. Cisco UCS C240 M7 stand-alone rack server connectivity with Cisco Nexus Switches



## **Cisco Intersight Configuration**

This section contains the following:

- <u>Claim Target</u>
- Pool Configuration
- Policy Configuration
- Template and Profile Configuration
- Install Operating System using Cisco Intersight

Cisco Intersight Infrastructure Service allows policy managed infrastructure configuration for ease of management, monitoring and Remediate issues and stay ahead with proactive awareness of Cisco UCS Infrastructure.

#### Tech tip

Please visit Intersight Help Center for more details: https://us-east-1.intersight.com/help/saas/home

This section highlights initial configuration required to claim a target in a new or existing Cisco Intersight account. Based on the requirement and intended configuration for Cisco Intersight managed Infrastructure either create new pools, policies, template, and profiles or leverage existing configuration for faster deployment. Github repositories for automated FlexPod deployment and configuration can be found here: <a href="https://github.com/orgs/ucs-compute-solutions/repositories">https://github.com/orgs/ucs-compute-solutions/repositories</a>

#### Claim Target

This procedure details how to claim a Cisco UCS standalone server using Cisco Intersight.

**Step 1.** Log into CIMC web UI <u>https://<cimc\_mgmt\_ip</u>> and enter your username and password.

**Step 2.** Go to Admin > Device Connector.

	2	Et dudu Cisco	Integrated Management Controlle	r	_		¥	☑ 0 admin@10
	*	🕈 / Chassis / Sum	mary 🛨				Refresh Host Power	Launch vKVM Ping
Chassis	٠	Server Proper	ties	Cisco Integrated I	Management Controller (Cisco	o IMC) Information		
Compute		Product Name:	UCS C240 M7SN	Hostname:	C240-WZP270500PV			
Networking	۲	Serial Number:	WZP270500PV	IP Address:	10.29.148.55			
Storage		UUID:	0GSC-G240-M7SN 19643E1C-2ACC-4C8D-A893-0818E6BA67E1	Firmware Version:	4.3(2.230207)			
Admin		BIOS Version: Description:	C240M7.4.3.2a.0.0710230213 HPC-Node2	Current Time (UTC): Local Time:	Wed Oct 25 20:50:09 2023 Wed Oct 25 13:50:09 2023 PDT -0700 (NTP)			
User Management		Asset Tag:	Unknown	Timezone:	America/Los_Angeles	Select Timezone		
Networking								
Communication Services		Chassis Statu	S	Server Utilization				
Security Management		Power	State: On	(%)				
Event Management		Post Completion	Status: Completed	100		Overall Utilization (%)		
Firmware Management		Overall Server : Tempe	status: 🍯 Good	80 -		Memory Utilization (%)		
Utilities		Overall DIMM	Status: 🗹 Good	60 -		IO Utilization (%)		
Device Connector Device Connector		Power Su	pplies: 🗹 Good	50 40				
		Locato	r LED: Off	30-20-				
		Overall Storage	Status: 🗹 Good	10				
				0	Server			

**Note:** This is the first step. In general, processes should have multiple procedures, and procedures should have multiple steps.

🗲 📲 Cisco Integrated Management Controller 🕴 🖂	admin@10.155.164.115 - C240-WZP27	010H3G 🛱
Please note: Intersight Infrastructure Services license is required with this server. Learn More.		
n / Admin / Device Connector * Refresh   Host Power   Launch v	KVM   Ping   CIMC Reboot   Locator L	ED   0 0
The Device Connector is an embedded management controller that enables the capabilities of Cisco intersight, a cloud-based management platform. For detailed information about configuring the device connector, please visit Help Center		
Device Connector	Settings	💭 Refresh
Device Connector	Device ID WZP27010H3G Claim Code 42DCE8EE2B2E	120 120
Not Claimed  The connection to the Cisco intensight Portal is successful, but device is still not claimed. To claim the device open Cisco intensight, create a new account and follow the guidance or go to the Targets page and clok Claim a New Device for Open Intensight Intensight		
1.0.11-0130		

**Step 3.** Update settings input as appropriate and click Save.

Settings	
General	
DNS Configuration	When this option is ON, you can claim this system and leverage the capabilities of Cisco Intersight. If it is OFF, no communication will be allowed to Cisco Intersight. Learn More
Proxy Configuration	Device Connector
Certificate Manager	Access Mode
	<ul> <li>Read-only</li> <li>Allow Control</li> <li>Configuration from Intersight only O</li> <li>Tunneled vKVM</li> </ul>

Step 4. Copy Device ID and Claim code to be entered while claiming a target in Cisco Intersight.

**Step 5.** Log into Cisco Intersight; go to System > Targets. Click Claim a new Target.

≡	disd: Intersight	🖥 System 🗸	Q Search	0 4 000	💴 💿 🛛 🔍
0	Settings	Targets		9	Claim a New Target
	Targets Software Repository	X All Targets  +	🖂 31 items found	10 → per page K C	1 of 4 ⊃ Э
	Tech Support Bundles Audit Logs Sessions	Connection Connected 31	ets by Types • Standalone M6/M7 31	• Cisco Systems, Inc. 31	ж
	Litenang	Name : Status	: Type : Claime	ed Time 🗧 Claimed By	: Ø

Step 6. Select Cisco UCS Server (standalone) in Compute/Fabric section. Click Start.

≡	، البنان Intersight	System V	Q Search	D ⊗ ⊄	Q 0 🚺 💿   A
0	Settings Admin ^ Targets Software Repository	← Targets Claim a New Target	t Select Target Type	1	
	Tech Support Bundles Audit Logs Sessions Licensing	Filters         Available for Claiming         Categories         All         Cloud	Q. Search         Compute / Fabric         Image: stands         Cisco UCS Server (Standalone)         Cisco UCS C890         Red	-deale CCS Domain ght Managed)	cieco Cisco UCS Domain (UCSM Managed)
		Cancel			Start

**Step 7.** Enter Device ID and Claim Code copied from Cisco CIMC for the standalone server to claim in the Cisco Intersight.

≡	illisles Intersight 📃 📲 s	System V	Q Search	📄 O 4 D 🛛 🗠	A \ @ \
0 ()	Settings Admin ^	← Targets Claim a New Targ	et		
	Targets	General			
	Software Repository Tech Support Bundles	Device ID * WZP27010H3G ◎	Claim Code * 42DCE8EE2B2E		
	Audit Logs Sessions	Resource Groups			
	Licensing	i Select the Resource G type is 'All'. The claime	roups if required. However, this selection is not Id target will be part of all Organizations with th	mandatory as one or more Resource e Resource Group type 'All'.	Group
		□ Name	0 items found Usage	50 ✓ per page ເ∢ < 0 of 0 > > Description	
			NO ITEMS AVAILABLE		
		Back Cancel			Claim

Cisco CIMC and Cisco Intersight WebUI reporting Cisco UCS Rack Server claimed and connected is shown below:

🔹 📲 🔐 Cisco Integrated Management Controller	_	* 🗹 0	admin@10.155.164.115 - C240-WZP27010H3G 🏾 🌣
A / Admin / Device Connector *		Refresh   Host Power   Launch	vKVM   Ping   CIMC Reboot   Locator LED   🙆 🄇
The Device Connector is an embedded management controller that enables the capabilities of Cisco Intersight, a	a cloud-based management platform. For detailed information	about configuring the device connector, please visit Help Center	
Device Connector			🛞 Settings 🛛 💭 Refresh
Device Connector		intersight	Device ID WZP27010H3G E Claimed to Account SJC2-UCS-AI ① Unclaim
Claimed			
1.0.11-3136			

≡	tiliali Intersight	🖥 System 🗸		
0	Settings	Targets		
	Targets	★ All Targets		
	Software Repository	🖉 📋 📔 🍳 Add Filter		
	Tech Support Bundles	Connection	Top Targets by Types	Vendor
	Sessions	Not Connected 7	39 • Standalone M6/M7 39	39 • Cisco Systems, Inc. 39
	Licensing	Name		Claimed Time
		C240-WZP27010H3G	© Connected Standalo	ne M7 Ser 2 minutes ago

#### **Pool Configuration**

## Tech tip

For more information on licensing requirements for Infrastructure Services, see Infrastructure Services License.

You can either create the required pools and policies to attach to a server profile or create them as progressing through the server profile/template creation.

**Step 1.** Log into Cisco Intersight. Go to Infrastructure Service.





≡	cisco Intersight	<sub>o</sub> ≉⊜ Infr	astructure Service $$		Q Search	⊘ ⊄ ₽ @   A
:¢:	Overview		Pools			
( <b>Q</b> )	Operate	<ul><li>✓</li><li>✓</li></ul>	ools Reserved Identifiers	VRFs		
୍	Analyze					Circote Deal
	Configure	^				Create Puor
	Profiles		<u>* All Pools ©</u> +	ter	🕒 Export 7 items found 10 ~	perpage 📧 < 1 of 1 🔉 河
	Templates					
	Policies		IP X		UUID X	
	Pools		4 • Used 4	(1152) • Used 4	(128) • Used 2 • Available 128	

**Step 3.** Select Resources. Click Start. Enter a name for the new Resource Pool. Select the Target Platform to add in the resource pool. Select by filtering the set of nodes to be part of the resource pool. For example, UCSC-C240-M7 as shown below:

Resource Pool						
General .	Pool Det Set configurati	cails on for the resource po	ol.			
Pool Details	<b>і</b> тн	ne only resource type a	vailable for pool o	creation is Server.		
	Resour	ce Selection				
		G	21 items found	50 v per pag	ge K < _1_of1 >	≥ \$
	Q	Model UCSC-C240-M2	Add Filter			
		Name ‡	Health ‡	Manage 💲	Model ‡	Memo
		C240-WZP27100	Healthy	10.29.148.43	UCSC-C240-M7SX	512.(
		C240-WZP27100	Healthy	10.29.148.45	UCSC-C240-M7SX	512.(
		C240-WZP27100	Healthy	10.29.148.46	UCSC-C240-M7SX	512.(
		C240-WZP27020	Healthy	10.29.148.42	UCSC-C240-M7SX	512.(
			A Healthy	10 29 1/18 //		512 (
<	Cancel					Back Save

Step 4. Create the IP Pool for KVM access as shown below:

IP Pool			
General	Configure IPv4 Pool		
IPv4 Pool Details	i Previously saved parame	eters cannot be changed. You can find Cisco recommendations a	t Help Center.
IPv6 Pool Details	Configuration		
	Netmask *	Gateway	
	255.255.255.0	° 10.29.148.1	
	Primary DNS 171.70.168.183	<ul> <li>Secondary DNS</li> </ul>	
	IP Blocks		
	From	Size	
	10.29.148.77	<sup>©</sup> 64	Ĵ = +
<	Close		Back Next

#### **Policy Configuration**

This section provides the screenshots where input is required to complete the policy creation. The process remains the same, such as selection of organization, entering name for the policy, tags, and description.

Step 1. Go to Policies. Select type of policy to create.

Select Policy Type				
Filters	Q, Search			
<ul> <li>Platform Type</li> <li>All</li> <li>UCS Server</li> <li>UCS Domain</li> <li>UCS Chassis</li> <li>HyperFlex Cluster</li> <li>Kubernetes Cluster</li> </ul>	<ul> <li>Backup Configuration</li> <li>Replication Network Configuration</li> <li>Adapter Configuration</li> <li>Add-ons</li> <li>Add-ons</li> <li>Auto Support</li> <li>BIOS</li> <li>Boot Order</li> <li>Certificate Management</li> <li>Container Runtime</li> <li>Device Connector</li> </ul>	<ul> <li>Firmware</li> <li>Flow Control</li> <li>HTTP Proxy</li> <li>Http Proxy Policy</li> <li>IMC Access</li> <li>IPMI Over LAN</li> <li>iSCSI Adapter</li> <li>iSCSI Boot</li> <li>iSCSI Static Target</li> <li>Kubernetes Version</li> </ul>	<ul> <li>Port</li> <li>Power</li> <li>SAN Connectivity</li> <li>SD Card</li> <li>Security</li> <li>Serial Over LAN</li> <li>SMTP</li> <li>SNMP</li> <li>SSH</li> <li>Storage</li> </ul>	
	Cancel			

Step 2. Select BIOS and click Start.

**Step 3.** We kept all settings as platform-default, except for the following parameters changes in the BIOS policy:

- LLC dead line Disabled
- Intel Virtualization Technology Disabled
- LLC prefetch Disabled
- Workload configuration Balanced

#### **Tech tip**

Selection of BIOS parameters determines the cluster optimization for performance or power saving or balanced of performance and power savings goal.

Please review Performance Tuning Best Practices Guide for Cisco UCS M7 Platforms: <u>https://www.cisco.com/c/en/us/products/collateral/servers-unified-computing/ucs-b-series-blade-servers/ucs-m7-platforms-wp.html</u>

Policies > BIOS > ucs-m7-bios				
General	Core Multi Processing all		Energy Performance performance	
2 Policy Details	Frequency Floor Override platform-default		CPU Performance enterprise	
	Power Technology performance		Demand Scrub platform-default	
	Direct Cache Access Support enabled		DRAM Clock Throttling Performance	
	Energy Efficient Turbo platform-default		Energy Performance Tuning platform-default	
	Enhanced Intel Speedstep(R) Technolog enabled	gy ∽ ⊙	Processor EPP Enable platform-default	
Policies > BIOS > ucs-m7-bios Edit				
Policies > BIOS > ucs-m7-bios Edit Seneral	Intel(R) VT disabled	II V O P	IO Error Enable platform-default	<b>v</b> ©
Policies > BIOS > ucs-m7-bios Edit © General 2 Policy Details	Intel(R) VT disabled DCU IP Prefetcher platform-default	✓ ○ P ✓ ○ P	IO Error Enable platform-default (TI Prefetch platform-default	<ul> <li>♥</li> <li>●</li> </ul>
Policies > BIOS > ucs-m7-bios Edit © General 2 Policy Details	Intel(R) VT disabled DCU IP Prefetcher platform-default LLC Prefetch disabled	<ul> <li>✓ ○</li> <li>✓ ○</li> <li>✓ ○</li> <li>✓</li> <li>✓</li></ul>	IO Error Enable olatform-default (TI Prefetch olatform-default ntel Memory Interleaving olatform-default	<ul> <li>•</li> <li>•</li> <li>•</li> <li>•</li> <li>•</li> <li>•</li> <li>•</li> <li>•</li> </ul>
Policies > BIOS > ucs-m7-bios Edit <ul> <li>General</li> <li>Policy Details</li> </ul>	Intel(R) VT disabled DCU IP Prefetcher platform-default LLC Prefetch disabled Package C State Limit platform-default		IO Error Enable olatform-default KTI Prefetch olatform-default ntel Memory Interleaving olatform-default Patrol Scrub olatform-default	<ul> <li>•</li> <li>•&lt;</li></ul>
Policies > BIOS > ucs-m7-bios Edit © General 2 Policy Details	Intel(R) VT disabled DCU IP Prefetcher platform-default LLC Prefetch disabled Package C State Limit platform-default Patrol Scrub Interval * platform-default		IO Error Enable olatform-default CTI Prefetch olatform-default ntel Memory Interleaving olatform-default Patrol Scrub olatform-default	<ul> <li>•</li> <li>•&lt;</li></ul>

**Step 4.** Create Boot order policy. Select UCS Standalone Server. Select Boot Mode. Click Add Boot Device. Select LocalDisk from the drop-down list for "Add Boot Device." For the device name and Slot enter "MSTOR-RAID."

Policies > Boot Order					
Create					
	Configured Boot Mode ©				
General	Unified Extensible Firmware Interface (UEFI)	) Lega	су		
2 Policy Details	● Enable Secure Boot ©				
	Add Boot Device				
	– Local Disk (m2-localboot)		Enabled 🛛 🖻		
	Device Name * m2-localboot		Slot MSTOR-RAID		
	Bootloader Name		Bootloader Description		
	Bootloader Path				
<	Cancel		Back	Cre	eate

**Note:** Additional boot devices can be added as per the requirement.



**Step 5.** Create the SSH policy.

General	Policy Details Add policy details
	i This policy is applicable only for UCS Servers (Standalone)
	Enable SSH 0
	SSH Port
	22
	SSH Timeout(seconds)
	1800 🗘 💿



<ul> <li>General</li> <li>Policy Details</li> </ul>	Policy Details         Add policy details         Image: Server (Standalone)         Image: Server (Standalone)         Image: Server (Standalone)	omain
	Enable NTP ©	
	NTP Servers * 72.163.32.44 • +	
	Timezone America/Los_Angeles v	

**Step 7.** Create the Virtual KVM policy.
General	Policy Details Add policy details
2 Policy Details	All Platforms UCS Server (Standalone) UCS Server (FI-Attached)
	Enable Virtual KVM 💿
	Max Sessions * <u>4 〔3 ○</u> 1 - 4
	Remote Port * 2068 Ĵ ○ 1 - 65535
	Enable Video Encryption ○
	Enable Local Server Video 🜼
	Allow Tunneled vKVM ©

**Step 8.** Create the Storage policy to create RAID 1 on two M.2 SATA SSD with boot optimized RAID controller. Select M.2 RAID configuration. From the drop-down list select MSTOR-RAID-1(MSTOR-RAID).

	All Platforms	UCS Server (Standalone)	UCS Server (FI-Attached)
General Configuration			
Use JBOD drives for Virtual Drive creation ◎			
Unused Disks State JBOD			
Default Drive State			
Secure JBOD Disk Slots			
M.2 RAID Configuration			
Slot of the M.2 RAID controller for virtual drive creation MSTOR-RAID-1 (MSTOR-RAID)			

# Template and Profile Configuration

**Step 1.** In Cisco UCS Infrastructure Services page, go to Templates. Click Create UCS Server Profile Template.

≡	''''' Intersight	ိုး၊	nfrastructure Service	~	Q	Search		(	୭	¢,	Q 이	<u>A</u> 1	0	<u>ନ</u>
:Ø:	Overview		Template	es										
Ø	Analyze		UCS Server Profile	e Templates										
( <b>Q</b> )	Operate	$\sim$												
	0								Cre	eate UC	S Serve	r Profile	Templa	te
	Configure	^												
	Profiles		* All UCS Server F	Prof ⊕ +										
	Templates			Add Filter			G	3 items found	± 1	0 ~ pe	r page	K < _	1 of 1	
	Policies		Name	÷	Usage 🗘	Target Platf	. ÷	Description			La	ist Upda	te :	Ş

Step 2. Enter a name for the Server Profile Template and select the Target Platform.

← Templates Create UCS Server Profile Template						
1 General	General					
2 Compute Configuration	Enter a name, description, tag and select a platform for template.	the server profile				
3 Management Configuration	Organization * default					
4 Storage Configuration						
5 Network Configuration	Name * ucs-c240m7-template					
6 Summary						
	Target Platform ◎ ● UCS Server (Standalone) ○ UCS Server (Fl-Attach	ed)				
<	Close	Next				



# **Create UCS Server Profile Template Compute Configuration** General $\langle \rangle$ Create or select existing Compute policies that you want to associate with **Compute Configuration** this template. 2 BIOS 🥑 ucs-m7-bios 🗐 (3) Management Configuration Boot Order (4) Storage Configuration Firmware 🛛 ucs-m7-firmware 📋 **Network Configuration** (5) Persistent Memory Summary Thermal Virtual Media ucs-vmedia Close Back Next ← Templates **Create UCS Server Profile Template**

LDAP	
Local User	
Network Connectivity	
NTP	✓ ucs-ntp
Serial Over LAN	
SMTP	
SNMP	
SSH	✓ ucs-ssh
Syslog	
Virtual KVM	✓ ucs-vkvm
Close	Back Next
	LDAP Local User Network Connectivity NTP Serial Over LAN SMTP SNMP SSH Syslog Virtual KVM

Create UCS Server P	rofile Template
General	Storage Configuration Create or select existing Storage policies that you want to associate with
Compute Configuration	this template.
Management Configuration	Drive Security
4 Storage Configuration	SD Card
5 Network Configuration	Storage Storage
6 Summary	
<	Close Back Next



← Templates							
Create UCS Server Profile Template							
	rembio	ale					
General	Target	: Platform <b>erver</b>					
Compute Configuration	(Standalone)						
Management Configuration	ement	Storage	Network	Errors/Warnings			
Storage Configuration		Configuration	Configuration	(0)			
Network Configuration	BIOS			ucs-m7-bios 🗐			
Cummary	Boot O	rder		ucs-boot 🗐			
Summary	Firmwa	ire		ucs-m7-firmware 🗐			
	Virtual	Media		ucs-vmedia 🗐			
<	Close		Bac	ck Derive Profiles			



UCS Server Profile Templates > ucs-c240m7-	template	
Derive		
	ucs-c240m7- default template	
1 General		
2 Details		
	(Standalone)	
3 Summary		
	^ Server Assignment	
	Assign Now From a Resource Pool Serial Number	Assign La
	$ \begin{array}{ccc} \hline \rightarrow & 1 \text{ items found} & 10 \lor \text{ per page } \ltimes & \swarrow & 1 & \text{of } 1 \\ \hline & & & & \\ \hline & & & & \\ \hline & & & & \\ \hline & & & &$	
	୍ଦ୍ର Add Filter	
	N. C. U. C. Health C. M. C. UCS.	s
	C24 CDIP 🕑 Healthy UCS	v
<	Cancel	Next

**Step 6.** Edit the name for the server profile(s) to be derived from the template.

UCS Server Profile Templates > ucs-c240n	n7-template		
General	default	✓ UCS Server (Standalon	
3 Summary	Description <	<u>∡</u> = 1024	
	A Derive           1         Name *           C240M7-HPCAI-1	Organization * default ∽	Assig <b>C240-</b>
			WZP27 010H3 G
<	Close	Bac	k Next

Step 7. Click Deploy Server Profile. Monitor the Server profile deployment task.

<ul> <li>Requests</li> <li>Deploy Server Profile</li> </ul>		×
Details	Execution Flow	
Status	⊘ Deploy Boot Order Policy	
Success	O Deploy Storage Policy	
Name	⊘ Deploy Device NTP Policy	
Deploy Server Profile	O Deploy BIOS Policy	
ID	⊘ Deploy SSH Policy	
6539bbda696f6e3101ee76e2 Target Type	Opploy Virtual KVM Policy Tunneled vKVM configuration is disabled for the account.	
Target Name	Validate Storage Policy Completed	
Source Type	Some Statistics States	
Server Profile	⊘ Wait for Storage subsystem initialization.	
Source Name	⊘ Validate NTP Policy	Oct 25, 2023 6:07 PM

## Install Operating System using Cisco Intersight

### **Prerequisites**

Create the NFS or HTTPS file share location to be consumed for the Operating System, Cisco UCS SCU, and the Cisco UCS HUU repository.

**Step 1.** Download ISO and copy the path location to be added in Software Repository tab.

Step 2. Log into Cisco Intersight. Go to System > Software Repository.

٥	Settings	oftware Repository						
U	Admin ^ Targets	Firmware Links OS Image Links	SCU Links OS Configuration Files					
	Software Repository			Add Firmware Link				
	Tech Support Bundles							
	Audit Logs	+ All Firmware Links ⊗ +						
	Sessions		🕒 3 items found 10 🗸	• per page				
	Licensing	Q Add Filter ☐ File Name  \$	Version	File Location 🖇				
			4.3(2.230207) UCSC-C220-M7S, UC (6)	https://10.29.148.20/iso/ucs ····				
		ucs-c240m6-huu-4.3.2.2	4.3(2.230207) UCSC-C240-M6S, UC (5)	https://10.29.148.20/iso/ucs •••				
		ucs-c240m7-huu-4.3.2.2	4.3(2.230207) UCSC-C240-M7S, UC (6)	https://10.29.148.20/iso/ucs ····				
				K く <u>1</u> of 1 > 洌				

Step 3. Go to OS Image Links and click Add OS Image Link.

Softwar	Software Repository							
Firmware Links	OS Image Links	SCU Links	OS Configuration Fil	les				
				Add OS Image Link				
* All OS Ima	nge Links ⊗ + ⊘   er		🗗 4 items found	10 ∨ per page				

**Step 4.** Select NFS or CIFS or HTTP/s, enter file location, username, and password.

Software Repository $>$ OS Image Links <b>Add</b>	
<ol> <li>General</li> <li>Details</li> </ol>	Organization * default ~ NFS CIFS HTTP/S File Location * https://10.29.148.20/iso/ubuntu-22.04-live-server-amd64.is <sup>©</sup>
	Username root © Password © 0
<	Cancel Next

Step 5. Enter the Details.

Software Repository $\rightarrow$ OS Image Links Add			
<ul> <li>General</li> <li>Details</li> </ul>	<b>Details</b> Review Operating System imag Operating System image. Name * Ubuntu-22.04LTS	ge detail ©	s, modify as required, and save the
	Vendor * Ubuntu Set Tags	<b>*</b>	Version * Ubuntu Server 22.04 LTS ~ Description
<	Cancel		Back Add

**Step 6.** Go to SCU Links page System > Software Repository. Click Add SCU Link.

≡	'disco' Intersight	∎Ē Sy	∕stem ∨		Q Search		$\oslash$	₽	Q 이	<u>A</u> 1	0	R
o	Settings		Softwar	e Reposit	ory							
	Admin /	^	Firmware Links	OS Image Links	SCU Links	OS Configuration I	Files					
	Targets											
	Software Repository									Add	SCU Lin	k
	Tech Support Bundles											
	Audit Logs		* All SCU Li	nks ⊕ +								
	Sessions					2 items found	10 ~	per pa	ige 🔣 <	1 of	1 > স	
			୍କୁ Add Filt	er								

Step 7. Enter the File Location, Username and Password. Click Next.





<ul> <li>General</li> <li>Details</li> </ul>	<b>Details</b> Review Server Configuration Utility in save the Server Configuration Utility	mage details, modify as required, and image.
	Name *	
	ucs-m7-scu-6.3.1b	
	Version *	Supported Models *
	6.3.1b O	UCSC-C240-M7,UCSC-C220-M7 <sup>©</sup>
	Set Tags	Description
<	Cancel	Back Save

**Step 9.** Go to the OS Configuration Files tab. Add the OS configuration file for Operating System Installation (optional).

≡	the Intersight	System 🗸	Q Search		⊘ ⊄	Q 🛛 🔺	ଡ
o	Settings	Software Reposit	ory				
	Admin ^	Firmwara Linka OS Imaga Linka	COLL inka	OS Configuration Fil			
	Targets	Firmware Links OS image Links	SCO LINKS		uration Files		
	Software Repository					Add OS Configu	iration File
	Tech Support Bundles						
	Audit Logs	× All OS Configuratio ⊗ +					
	Sessions			🕒 2 items found	10 ~ per	oage K < 1 o	f1 🔉 河

**Step 10.** Go to Infrastructure Service > Servers. Select system(s) to perform Install Operating System. Rightclick on the ellipses and select Install Operating System.

ښ: ح	Overview Analyze	Servers	
		¥ ΔII Servers ⋒ →	
( <b>Q</b> )	Operate ^	··· ⊘ ··· ○ · ○ · ○ · ○ · ○ · ○ · ○ · ○ · ○ ·	of 1 🕞 河
	Servers	Power > 175X' × Add Filter	×
	Chassis	System >	
	Fabric Interconnects	Profile > Power HCL Status Models	
	HyperFlex Clusters	Install Operating System     7     • C240 M       Upgrade Firmware     7     • C240 M	и7sx 7 <-
	Integrated Systems	Set License Tier	
<b>,</b> G	Configure ^	Vame   Constraints  Constraints	del 🖗
	Profiles	C240-WZP27020EFR C Healthy 10.29.148.42 UCS	SC-C2 ····
	Tomplatos	C240-WZP27100DJZ C240-WZP27100DJZ C240-WZP27100DJZ C240-WZP27100DJZ C240-WZP27100DJZ C240-WZP27100DJZ	SC-C2 ***
	remplates	C240-WZP27100DJ4 (@ Healthy) 10.29.148.44 UCS	SC-C2
	Policies	C240-WZP27100DJE C240-WZP27100DJE C240-WZP27100DJE C240-WZP27100DJE	SC-C2 ····
	Pools	☑         ○         C240-WZP27100DJ5         ☑         Healthy         10.29.148.46         UCS	SC-C2. •••

**Step 11.** The selected system(s) are already part of the Operating System Install task. Edit the list if required. Click Next.



Step 12. Select the OS Image Link for the intended operating system to be installed.

OPERATE > Servers						
Install Operating System						
General		i	Selected servers belon organization: 'default'. ' install Operating System	g to si ⁄ou ca m from	ngle common n choose to n one of the	
2 Operating System		common organizations. Learn more at Help Center.				
3 Configuration		4 item	s found 10 ∨ per pa	ge 📧	] < 1 of 1 > >	Ę
4 Server Configuration Utility		Q /	Add Filter			
5 Installation Target			Name	¢	File Location	
6 Summary			rhel-9.1		https://10.29.148.20	
Summary			ubuntu-22.04.2		https://10.29.148.20	
			Ubuntu22.04.1		https://10.29.148.20	
		٢	ubuntu-22.04-LTS		https://10.29.148.20	
		Select	ed			_
	< Cancel				Back	Next

**Step 13.** Enter the configuration details for the Operating System to be installed as shown in the screenshot below. Repeat these steps for all system(s).

OPERATE > Servers Install Operating System							
	IP Configuration						
General	IPv4 IPv6						
Operating System	IP Address *	Netmask *					
	10.29.148.201 <sup>©</sup>	255.255.255.0					
3 Configuration							
4 Server Configuration Utility	Gateway *						
,	10.29.148.1						
5 Installation Target							
6 Summary	Name Server *	Hostname *					
	171.70.168.183 ©	hpc-node1 O					
	Network Device						
	eno5 0						
<	Cancel	Back Next					

Step 14. Select the Server Configuration Utility Image.

OPERATE > Servers Install Operating System						
General						
Operating System	Server Configuration Utility images are filtered based on the Operating System image					
Configuration						
4 Server Configuration Utility	2 items found 10 ∨ per page K < 1 of 1 > > ₹					
5 Installation Target	Name					
6 Summary	ucs-m6-scu-6 https://10.29.148.20/iso/ucs-sc					
	ucs-m7-scu-6 https://10.29.148.20/iso/ucs-sc					
	Selected Show Selected Unselect All 📧 🔄 1 of 1					
<	Cancel Back Next					

Step 15. Select the Installation Target. We selected M.2 VD from the drop-down list.



Step 16. Review the Operating System Installation Summary. Click Install.



Step 17. Review the Installation workflow in execution.

# Requests > Operating System Install Operating System Install on Cisco UCS Server Details Execution Flow

Progress -

Track OS Install Preparation Progress 'Mapping OS ISO in progress'

 Initiate Operating System Installation Operating System installation initiated.

⊘ Handle Staged Policies on IMM Server View Execution Flow

Retrieve Server Configuration
 Server configurations retrieved successfully

 Validate Install Configuration Configuration validated.

 Process Workflow Input Task Workflow Inputs processed.

Prepare Operating System Install Configuration Configuration file is prepared for Operating System: Ubuntu Server 22.04.1 LTS, Configuration Source: Cisco Template.

Status

Name Operating System Install on Cisco UCS Se...

ID 64dbe912696f6e3101a6c93b

Target Type Rack Server

Target Name C240-WZP270500PF

Source Type Rack Server

Source Name C240-WZP270500PF

Initiator hardipat@cisco.com

Start Time Aug 15, 2023 2:07 PM

End Time

Duration

8 m 59 s

Organizations

default

≡	cisco Inte	ersight	C240-WZP270500PF   KVM Console	UCSC-C240-M7SN WZP270500PF
D	Console			Checking SCU mode Starting OS Installation Process
	File			Receiving OS Answer File and Config file Starting Non Interactive OS Installation
	View			Installing OS ubuntu22041x64
8	Macros			Clearing hard disk
×	Tools			Unmounting SCU ISO Unmap SCU ISO and map OS ISO (Linux Ubuntu 22.04.1) to continue installation
Ċ	Power			Preparing hard disk Extracting initrd
	Boot Device			Creating initrd
۵	Virtual Media		Create Image	
٩	Chat		vKVM-Mapped vDVD	
			vKVM-Mapped vHDD	
			vKVM-Mapped vFDD	
			≜ CISCO_Utils	

	Q Search 🥹 💽 🕫 🗘	 0	R
Requests > Operating System Install Operating System Install or	I Cisco UCS Server		×
Details	Execution Flow		
Status © Success	Set Server Power State     Server Power cycled successfully		
Name InstallOSIMM	<ul> <li>Redeploy Server Profile</li> <li>Server profile deployed successfully.</li> </ul>		
IP	⊘ Wait for OS to boot		
64dbe911696f6e3101a6c8d0	Monitor Operating System Installation     Operating System installation completed.		
Target Type Rack Server	Clean Operating System Configuration Files     Operating System configuration file cleanup completed		
Target Name C240-WZP27060119	Track OS Install Preparation Progress     Operating System install preparation completed		
Source Type			
Rack Server	<ul> <li>Initiate Operating System Installation Operating System installation initiated.</li> </ul>		
Source Name C240-WZP27060119	Prepare Operating System Install Configuration Configuration file is prepared for Operating System: Ubuntu Server 22.04.1 LTS, Configuration Source: Cisco Template.		
hardipat@cisco.com	Validate Install Configuration     Configuration validated.		
Start Time			
Aug 15, 2023 2:07 PM	Handle Staged Policies on IMM Server View Execution Flow		
End Time Aug 15, 2023 2:30 PM	Retrieve Server Configuration     Server configurations retrieved successfully		
Duration 23 m 24 s	Process Workflow Input Task     Workflow Inputs processed.		

	cisco Intersight	C240-WZP270500PF   KVM Console UCSC-C240-M7SN WZP270500PF
	Console	Ubuntu 22.04.1 LTS c240m7–5 tty1
	File	Hint: Num Lock on
۲	View	
8	Macros	c240m7-5 login: _
×	Tools	
$\bigcirc$	Power	
$\uparrow$	Boot Device	
٥	Virtual Media	
Ð	Chat	

# **Post-OS Configuration**

This section contains the post-OS configuration steps:

- OS Configuration
- <u>Ansible Automation</u>

#### **OS Configuration**

**Step 1.** Log into the Ubuntu OS management IP address configured during the Cisco Intersight based Install Operating System using the SSH client. Enter the username "ubuntu" and the password entered while setting up the custom configuration:

\$ ssh ubuntu@10.29.148.171

Edit /etc/hosts

\$ cat /etc/hosts

127.0.0.1 localhost

127.0.1.1 hpc-node1

- 10.29.148.171 hpc-node1
- 10.29.148.172 hpc-node2
- 10.29.148.173 hpc-node3
- 10.29.148.174 hpc-node4
- 10.29.148.175 hpc-node5
- 10.29.148.176 hpc-node6
- 10.29.148.177 hpc-node7
- 10.29.148.178 hpc-node8

# The following lines are desirable for IPv6 capable hosts

::1 ip6-localhost ip6-loopback

fe00::0 ip6-localnet

ff00::0 ip6-mcastprefix

ff02::1 ip6-allnodes

ff02::2 ip6-allrouters

**Note:** If it's not already installed, the following steps require openssh-server to be installed using "sudo apt install -y openssh-server"

Step 2. Add a new user:

\$ adduser <username>

Adding user `<username>' ...

Adding new group `<username>' (1001) ...

Adding new user `<username>' (1001) with group `<username> ...

Creating home directory `/home/<username>' ...

Copying files from `/etc/skel' ...

New password: <Password!>

Retype new password: <Password!>

passwd: password updated successfully

Changing the user information for <username>

Enter the new value, or press ENTER for the default

Full Name []: FirstName LastName

Room Number []:

Work Phone []:

Home Phone []:

Other []:

Is the information correct? [Y/n] Y

\$ usermod -aG sudo <username>

\$ su - <username>

To run a command as administrator (user "root"), use "sudo <command>".

See "man sudo\_root" for details.

**Step 3.** Setup a password-less login:

This process needs to be completed on each node so that all nodes can be accessed without password for HPC cluster test as documented in following section.

\$ ssh-keygen -N " -f ~/.ssh/id\_rsa

\$ for i in {1..8}; do echo " copying hpc-node\$i"; ssh-copy-id -i /home/ubuntu/.ssh/id\_rsa.pub ubuntu@HPC-Node\$i; done;

#### **Ansible Automation**

Step 1. Install ansible:

\$ sudo apt update

\$ sudo apt install software-properties-common

\$ sudo add-apt-repository --update ppa:ansible/ansible --> Press Enter when prompted

\$ sudo apt update

\$ sudo apt install -y ansible-core ansible

\$ ansibleversion					
ansible [core 2.15.4]					
config file = /etc/ansible/ansible.cfg					
configured module search path = ['/home/hardipat/.ansible/plugins/modules', '/usr/share/ansible/plugins/modules']					
ansible python module location = /usr/lib/python3/dist-packages/ansible					
ansible collection location = /home/hardipat/.ansible/collections:/usr/share/ansible/collections					
executable location = /usr/bin/ansible					
python version = 3.10.12 (main, Jun 11 2023, 05:26:28) [GCC 11.4.0] (/usr/bin/python3)					
jinja version = 3.0.3					
libyaml = True					
Step 2. Edit /etc/ansible/hosts:					
\$ sudo vi /etc/ansible/hosts					
[hpcnodes]					
hpc-node1 ansible_host=10.29.148.171					
hpc-node2 ansible_host=10.29.148.172					
hpc-node3 ansible_host=10.29.148.173					
hpc-node4 ansible_host=10.29.148.174					
hpc-node5 ansible_host=10.29.148.175					
hpc-node6 ansible_host=10.29.148.176					
hpc-node7 ansible_host=10.29.148.177					
hpc-node8 ansible_host=10.29.148.178					
[all:vars]					
ansible_python_interpreter=/usr/bin/python3					
Step 3. Test ansible:					
\$ ansible-inventorylist -y					
all:					
children:					
admin:					
hosts:					
10.29.148.22:					
ansible_python_interpreter: /usr/bin/python3					

hpcnodes: hosts: hpc-node1: ansible\_host: 10.29.148.171 ansible\_python\_interpreter: /usr/bin/python3 hpc-node2: ansible\_host: 10.29.148.172 ansible\_python\_interpreter: /usr/bin/python3 hpc-node3: ansible\_host: 10.29.148.173 ansible\_python\_interpreter: /usr/bin/python3 hpc-node4: ansible\_host: 10.29.148.174 ansible\_python\_interpreter: /usr/bin/python3 hpc-node5: ansible\_host: 10.29.148.175 ansible\_python\_interpreter: /usr/bin/python3 hpc-node6: ansible\_host: 10.29.148.176 ansible\_python\_interpreter: /usr/bin/python3 hpc-node7: ansible\_host: 10.29.148.177 ansible\_python\_interpreter: /usr/bin/python3 hpc-node8: ansible\_host: 10.29.148.178 ansible\_python\_interpreter: /usr/bin/python3 \$ ansible all -m command -a "uname -r" hpc-node2 | CHANGED | rc=0 >> 5.15.0-84-generic hpc-node4 | CHANGED | rc=0 >> 5.15.0-84-generic

#### Tech tip

To enable root login; edit "/etc/ssh/sshd\_config" as --> PermitRootLogin yes \$ sudo passwd root [sudo] password for ubuntu: New password: Retype new password: passwd: password updated successfully

#### Step 4. Setup NTP:

\$ ansible all -m command -a "sudo timedatectl set-timezone America/Los\_Angeles" \$ # ansible all -m command -a " sudo timedatectl set-ntp false" \$ ansible all -m command -a " sudo timedatectl set-time hh:mm" \$ ansible all -m command -a " sudo timedatectl set-time true" \$ ansible all -m command -a " sudo apt install ntp -y" **Step 5.** Edit /etc/ntp.conf and copy on all nodes: \$ vi /etc/ntp.conf pool 72.163.32.44 iburst \$ ansible all -m copy -a "src=/etc/ntp.conf dest=/etc/ntp.conf" Step 6. Start NTP service: \$ ansible all -m command -a "sudo systemctl start ntp" \$ ansible all -m command -a "sudo systemctl enable ntp" Step 7. Install required packages: \$ ansible all -m command -a "sudo apt-get update" \$ ansible all -m command -a "sudo apt-get install build-essential -y" \$ ansible all -m command -a "sudo apt install -y pip sshpass unzip -y" \$ ansible all -m command -a " sudo apt install environment-modules -y" \$ ansible all -m command -a "sudo apt install dkms -y" \$ ansible all -m command -a "sudo apt install make cmake -y" **Step 8.** Update Grub by editing /etc/default/grub: \$ ansible all -m shell -a "sed -i 's/GRUB\_\_CMDLINE\_LINUX\_DEFAULT=" [^" ]\*/& iommu=pt numa\_balancing=disable pci=realloc=off processor.max\_cstate=0/' /etc/default/grub"

\$ ansible all -m shell -a "update-grub"

Step 9. Disable Nouveau by running following commands:

\$ ansible all -m shell -a "bash -c "echo blacklist nouveau > /etc/modprobe.d/blacklist-nvidia-nouveau.conf" "

```
$ ansible all -m shell -a "bash -c "echo options nouveau modeset=0 >> /etc/modprobe.d/blacklist-nvidia-
nouveau.conf" "
```

\$ ansible all -m shell -a "update-initramfs -u"

#### **Tech tip**

The previous steps require a reboot:

\$ ansible all -m command -a "sudo reboot" **Step 10.** Disable firewall (or edit firewall configuration to allow NTP, NFS, other network traffic as appropriate):

\$ ansible all -m shell -a "sudo UFW disable"

Step 11. Disable SELinux:

\$ sudo vi /etc/selinux/config

SELINUX=disabled

\$ ansible all -m copy -a "src=/etc/selinux/config dest=/etc/selinux/config"

# Mellanox ConnectX-6 NIC Best Practice

This section highlights the steps required for the Mellanox ConnectX6-DX ehternet network interface card configuration for Ubuntu OS:

- Mellanox OFED Driver Installation
- <u>Configure Network Adapter Ports for Ubuntu</u>
- Mellanox ConnectX-6 NIC best practice for PFC, ECN and DSCP
- <u>Connect NetApp Storage provided FlexVolume(s) using NFS Mount</u>

#### **Mellanox OFED Driver Installation**

**Step 1.** Install Mellanox OFED for Mellanox ConnectX-6 DX Ethernet Network Interface Card. Download Mellanox OFED from the following URL:

https://www.mellanox.com/page/mlnx\_ofed\_eula?mtag=linux\_sw\_drivers&mrequest=downloads&mtype=ofed& mver=MLNX\_OFED-5.8-1.1.2.1&mname=MLNX\_OFED\_LINUX-5.8-1.1.2.1-ubuntu22.04-x86\_64.tgz

Step 2. Accept EUA to download Mellanox OFED Software:

\$ scp MLNX\_OFED\_LINUX-5.8-1.1.2.1-ubuntu22.04-x86\_64.tgz ubuntu@10.29.148.171:/home/ubuntu/

\$ ansible all -m copy -a "src=/home/ubuntu/ MLNX\_OFED\_LINUX-5.8-1.1.2.1-ubuntu22.04-x86\_64.tgz dest==/home/ubuntu/ MLNX\_OFED\_LINUX-5.8-1.1.2.1-ubuntu22.04-x86\_64.tgz"

\$ ansible all -m shell -a "tar xvf /home/ubuntu/ MLNX\_OFED\_LINUX-5.8-1.1.2.1-ubuntu22.04-x86\_64.tgz"

ansible all -m command -a "sudo /home/ubuntu/MLNX\_OFED\_LINUX-5.8-1.1.2.1-ubuntu22.04x86\_64/mlnxofedinstall --without-fw-update --force"

\$ ansible all -m command -a "sudo /etc/init.d/openibd restart"

\$ ansible all -m command -a "sudo reboot"

\$ ansible all -m command -a "ofed\_info -s"

hpc-node1 | CHANGED | rc=0 >>

MLNX_OFED_LINUX-5	5.8-1.1.2.1:				
hpc-node2   CHANGE	D   rc=0 >>				
MLNX_OFED_LINUX-5	5.8-1.1.2.1:				
Step 3. Start MST:					
\$ sudo mst start					
\$ sudo mst status -v					
MST modules:					
MST PCI module is I	not loaded				
MST PCI configurati	on module loaded				
PCI devices:					
DEVICE_TYPE	MST	PCI	RDMA	NET	NUMA
ConnectX6DX(rev:0)	/dev/mst/mt4125_pciconf0.1	27:00.1	mlx5_1	net-ens2f1np1	0
ConnectX6DX(rev:0)	/dev/mst/mt4125_pciconf0	27:00.0	mlx5_0	net-ens2f0np0	0
Tech tip					
GPU Direct RDMA and G	PU Direct Storage link:				
https://docs.nvidia.com/	datacenter/cloud-native/gpu-opera	tor/23.6.1/	<u>qpu-operator-</u>	rdma.html	

Once tested and validated next version of Cisco Validated Design will cover GPU Direct Storage.

#### **Configure Network Adapter Ports for Ubuntu**

Step 1. Run the following commands:

\$ ansible all -m command -a "sudo apt update"

\$ ansible all -m command -a "sudo apt install lldpad -y"

\$ ansible all -m command -a "sudo modprobe 8021q"

\$ ansible all -m command -a "sudo su -c 'echo "8021q" >> /etc/modules'"

\$ ansible all -m command -a " sudo apt install vlan -y"

**Step 2.** Edit /etc/netplan/00-installer-config.yaml to configure Mellanox NIC port with desired network configuration. For example, the following configuration is for Mellanox port1 (ens2f0np0) and port2 (ens2f1np1) connected to Cisco Nexus Switch A and B in Spine – Leaf architecture for data traffic.

\$ cat /etc/netplan/00-installer-config.yaml

# This is the network config written by 'subiquity'

network:

ethernets:

eno5: addresses: - 10.29.148.171/24 dhcp4: false nameservers: addresses: - 171.70.168.183 search: [] routes: - to: default via: 10.29.148.1 ens2f0np0: dhcp4: false ens2f1np1: dhcp4: false vlans: ens2f0np0.110: id: 110 link: ens2f0np0 mtu: 9000 addresses: - 192.168.110.171/24 routes: - to: 192.168.110.0/24 via: 192.168.110.1 metric: 100 ens2f1np1.160: id: 160 link: ens2f1np1 mtu: 9000 addresses: - 192.168.160.171/24

routes:

- to: 192.168.160.0/24 via: 192.168.160.1 metric: 100

version: 2

#### Mellanox ConnectX-6 NIC Best Practice for PFC, ECN and DSCP

**Step 1.** Enable ECN (Explicit congestion notification) priority 3: \$ ansible all -m command -a " sudo echo 1 > /sys/class/net/ens2f0np0/ecn/roce\_rp/enable/3" \$ ansible all -m command -a " sudo echo 1 > /sys/class/net/ens2f1np1/ecn/roce\_rp/enable/3" \$ ansible all -m command -a " sudo echo 1 > /sys/class/net/ens2f0np0/ecn/roce\_np/enable/3" \$ ansible all -m command -a " sudo echo 1 > /sys/class/net/ens2f1np1/ecn/roce\_np/enable/3" **Step 2.** Set CNP L2 egress priority: \$ ansible all -m command -a " sudo echo 6 > /sys/class/net/ens2f0np0/ecn/roce\_np/cnp\_802p\_prio" \$ ansible all -m command -a " sudo echo 6 > /sys/class/net/ens2f1np1/ecn/roce\_np/cnp\_802p\_prio" **Step 3.** Map CNP priority to Differentiated Services Code Point (DSCP): \$ ansible all -m command -a " sudo echo 48 > /sys/class/net/ens2f0np0/ecn/roce\_np/cnp\_dscp" \$ ansible all -m command -a " sudo echo 48 > /sys/class/net/ens2f1np1/ecn/roce\_np/cnp\_dscp" Step 4. Configure PFC (Priority-based Flow Control) - class 3: \$ ansible all -m command -a "sudo mlnx\_gos -i ens2f0np0 --pfc 0,0,0,1,0,0,0,0" \$ ansible all -m command -a " sudo mlnx\_gos -i ens2f1np1 --pfc 0,0,0,1,0,0,0,0" Step 5. Configure DSCP trust: \$ ansible all -m command -a "sudo mlnx\_qos -i ens2f0np0 --trust dscp" \$ ansible all -m command -a "sudo mlnx\_gos -i ens2f1np1 --trust dscp" Step 6. Enable ECN; edit /etc/sysctl.conf: \$ ansible all -m command -a "sudo sysctl -w net.ipv4.tcp\_ecn=1" **Step 7.** Set RoCE mode to v2: \$ ansible all -m command -a "sudo cma\_roce\_mode -d mlx5\_0 -p 1 -m 2" \$ ansible all -m command -a "sudo cma\_roce\_mode -d mlx5\_1 -p 1 -m 2" Step 8. Set DSCP value to 24 for RoCE traffic: \$ ansible all -m command -a "sudo cma\_roce\_tos -d mlx5\_0 -t 24" \$ ansible all -m command -a "sudo cma\_roce\_tos -d mlx5\_1 -t 24" Step 9. Map roce traffic to priority 3:

\$ ansible all -m command -a " sudo vconfig set\_egress\_map ens2f0np0.110 4 3"

\$ ansible all -m command -a "sudo vconfig set\_egress\_map ens2f1np1.160 4 3"

#### **Tech tip**

\$ ansible all -m command -a "sudo ip link set ens2f0np0.110 type vlan egress egress 0:0 1:1 2:2 3:3 4:4 5:5 6:6 7:7"

\$ ansible all -m command -a "sudo ip link set ens2f1np1.160 type vlan egress egress 0:0 1:1 2:2 3:3 4:4 5:5 6:6 7:7"

Step 10. Performance tuning on Mellanox NIC:

\$ ansible all -m command -a "sudo mlnx\_tune -p HIGH\_THROUGHPUT"

\$ ansible all -m command -a "sudo ip link set ens2f0np0.110 type vlan egress egress 0:0 1:1 2:2 3:3 4:4 5:5 6:6 7:7"

\$ ansible all -m command -a "sudo ip link set ens2f1np1.160 type vlan egress egress 0:0 1:1 2:2 3:3 4:4 5:5 6:6 7:7"

#### Connect NetApp Storage provided FlexVolume(s) using NFS Mount

Step 1. Install nfs-common on client server:

sudo apt install nfs-common -y

Step 2. Create mount directory:

\$ sudo mkdir /opt/hpc -p

\$ sudo mkdir /home/hpcdata -p

Step 3. Edit /etc/fstab to add permanent NFS mount:

\$ sudo vi /etc/fstab

192.168.110.5:/weather /opt/hpc nfs auto,noatime,nolock,bg,nfsvers=4.2,intr,tcp 0 0

192.168.110.5:/hpcdata /home/hpcdata/ nfs auto,noatime,nolock,bg,nfsvers=4.2,intr,tcp 0 0

Step 4. Mount NFS volume added in /etc/fstab:

\$ mount -a

Step 5. Validate mount point:

\$ df -h

# **NVIDIA GPU Configuration for HPC Workload**

This section highlights the steps required to configure NVIDIA GPU with Ubuntu OS and HPC workload:

- NVIDIA CUDA Installation on Ubuntu 22.04 LTS
- Post Installation Steps for NVIDIA CUDA
- <u>Sample CUDA Test</u>
- Install NVIDIA HPC SDK

# **NVIDIA CUDA Installation on Ubuntu 22.04 LTS**

Step 1. Verify You Have a CUDA-Capable GPU:

\$ ansible all -m shell -a "Ispci | grep -i nvidia"

hpc-node4 | CHANGED | rc=0 >>

99:00.0 3D controller: NVIDIA Corporation GA100 [A100 PCIe 80GB] (rev a1) hpc-node5 | CHANGED | rc=0 >> 99:00.0 3D controller: NVIDIA Corporation GA100 [A100 PCIe 80GB] (rev a1) hpc-node3 | CHANGED | rc=0 >> Step 2. Verify You Have a Supported Version of Linux: \$ ansible all -m shell -a "uname -m && cat /etc/\*release" hpc-node5 | CHANGED | rc=0 >> x86\_64 DISTRIB\_ID=Ubuntu DISTRIB\_RELEASE=22.04 DISTRIB\_CODENAME=jammy DISTRIB\_DESCRIPTION="Ubuntu 22.04.3 LTS" PRETTY\_NAME=" Ubuntu 22.04.3 LTS" NAME="Ubuntu" VERSION\_ID=" 22.04" VERSION=" 22.04.3 LTS (Jammy Jellyfish)" VERSION\_CODENAME=jammy ID=ubuntu ID\_LIKE=debian HOME\_URL=" https://www.ubuntu.com/" SUPPORT\_URL=" https://help.ubuntu.com/" BUG\_REPORT\_URL="https://bugs.launchpad.net/ubuntu/" PRIVACY\_POLICY\_URL=" https://www.ubuntu.com/legal/terms-and-policies/privacy-policy" UBUNTU\_CODENAME=jammy hpc-node4 | CHANGED | rc=0 >> **Step 3.** Verify the System Has gcc Installed: \$ ansible all -m shell -a "gcc --version" hpc-node5 | CHANGED | rc=0 >> gcc (Ubuntu 11.4.0-1ubuntu1~22.04) 11.4.0 Copyright (C) 2021 Free Software Foundation, Inc. This is free software; see the source for copying conditions. There is NO

warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.

hpc-node4 | CHANGED | rc=0 >>

gcc (Ubuntu 11.4.0-1ubuntu1~22.04) 11.4.0

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warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.

hpc-node2 | CHANGED | rc=0 >>

Step 4. Verify the system has the correct kernel headers and development packages installed:

\$ ansible all -m shell -a "uname -r"

hpc-node4 | CHANGED | rc=0 >>

5.15.0-84-generic

hpc-node5 | CHANGED | rc=0 >>

5.15.0-84-generic

**Step 5.** The kernel headers and development packages for the currently running kernel can be installed running the following:

\$ ansible all -m shell -a " sudo apt-get install linux-headers-\$(uname -r)"

Step 6. Download NVIDIA CUDA based on the requirement. Please refer to the screenshot below:

Operating System	Linux Windows
Architecture	x86_64 ppc64le arm64-sbsa aarch64-jetson
Distribution	CentOS     Debian     Fedora     KylinOS     OpenSUSE     RHEL     Rocky     SLES     Ubuntu
Distribution	WSL-Ubuntu
Version	20.04 22.04
Installer Type	deb (local) deb (network) runfile (local)

**Step 7.** Choose the Installation method.

Step 8. Remove Outdated Signing Key:

\$ ansible all -m shell -a "sudo apt-key del 7fa2af80"

**Step 9.** Add the pin file to prioritize CUDA repository:

\$ wget https://developer.download.nvidia.com/compute/cuda/repos/ubuntu2204/x86\_64/cudaubuntu2204.pin

\$ scp cuda-ubuntu2204.pin ubuntu@10.29.148.171:/home/ubuntu/

\$ ansible all -m copy -a "src=/home/ubuntu/cuda-ubuntu2204.pin dest=/home/ubuntu/cuda-ubuntu2204.pin"

\$ ansible all -m command -a "sudo mv /home/ubuntu/cuda-ubuntu2204.pin /etc/apt/preferences.d/cudarepository-pin-600 Step 10. Install local repository on file system:

\$ wget https://developer.download.nvidia.com/compute/cuda/12.2.2/local\_installers/cuda-repo-ubuntu2204-12-2-local\_12.2.2-535.104.05-1\_amd64.deb

\$scp cuda-repo-ubuntu2204-12-2-local\_12.2.2-535.104.05-1\_amd64.deb ubuntu@10.29.148.171:/home/ubuntu/

\$ ansible all -m copy -a "src=/home/ubuntu/cuda-repo-ubuntu2204-12-2-local\_12.2.2-535.104.05-1\_amd64.deb dest=/home/ubuntu/cuda-repo-ubuntu2204-12-2-local\_12.2.2-535.104.05-1\_amd64.deb"

\$ ansible all -m shell -a "sudo dpkg -i /home/ubuntu/cuda-repo-ubuntu2204-12-2-local\_12.2.2-535.104.05-1\_amd64.deb"

\$ ansible all -m command -a "sudo cp /var/cuda-repo-ubuntu2204-12-2-local/cuda-F73B257B-keyring.gpg /usr/share/keyrings/"

**Step 11.** Update the Apt repository cache:

\$ ansible all -m command -a " sudo apt-get update"

Step 12. Install CUDA SDK

\$ ansible all -m command -a " sudo apt-get install cuda -y"

**Step 13.** (optional) To include all GDS packages:

\$ ansible all -m command -a "sudo apt-get install -y nvidia-gds"

Step 14. Reboot the system:

\$ ansible all -m command -a "sudo reboot"

# Post Installation Steps for NVIDIA CUDA

Step 1. Environment Setup:

\$ ansible all -m shell -a "export PATH=/usr/local/cuda-12.2/bin\${PATH:+:\${PATH}}"

**Note:** When using the runfile installation method, the LD\_LIBRARY\_PATH variable needs to contain /usr/local/cuda-12.2/lib64 on a 64-bit system, or /usr/local/cuda-12.2/lib on a 32-bit system.

Step 2. To change the environment variables for 64-bit operating systems:

**Note:** The following paths change when using a custom install path with the runfile installation method.

\$ ansible all -m shell -a "export CUDA\_HOME=/usr/local/cuda-12.2"

\$ ansible all -m shell -a "export PATH=\${CUDA\_HOME}/bin:\${PATH}"

\$ ansible all -m shell -a "export LD\_LIBRARY\_PATH=\${CUDA\_HOME}/lib64:\$LD\_LIBRARY\_PATH"

**Note:** Recommended Actions – the following steps are recommended to verify the integrity of the installation.

**Step 3.** Verify the driver version:

\$ ansible all -m command -a " cat /proc/driver/nvidia/version"

hpc-node5 | CHANGED | rc=0 >>

NVRM version: NVIDIA UNIX x86\_64 Kernel Module 535.104.05 Sat Aug 19 01:15:15 UTC 2023

GCC version: gcc version 11.4.0 (Ubuntu 11.4.0-1ubuntu1~22.04)

hpc-node4 | CHANGED | rc=0 >>

NVRM version: NVIDIA UNIX x86\_64 Kernel Module 535.104.05 Sat Aug 19 01:15:15 UTC 2023

GCC version: gcc version 11.4.0 (Ubuntu 11.4.0-1ubuntu1~22.04)

hpc-node3 | CHANGED | rc=0 >>

Step 4. Run nvidia-smi command:

ubuntu@hpc-node1:~\$ nvidia-smi Thu Oct 26 19:08:06 2023									
NVID	IA-SMI	535.104	.05		Driver	Version:	535.104.05	CUDA Versio	on: 12.2
GPU   Fan 	Name Temp	Perf		Persist Pwr:Usa	tence-M age/Cap	Bus-Id	Disp.A Memory-Usage	Volatile   GPU-Util 	Uncorr. ECC Compute M. MIG M.
0   N/A 	NVIDIA 35C	A100 8 P0	OGB PCI	e 44W	0n / 300W	 0000000 4M	0:98:00.0 Off iB / 81920MiB	   0% 	0 Default Disabled
+									
Proc	esses: GI ID	CI ID	PID	Туре	Proces	ss name			GPU Memory Usage
No	running	proces	ses fou	nd					

#### Sample CUDA Test

Step 1. Based on github for cuda-samples: <u>https://github.com/NVIDIA/cuda-samples:</u>

hpc-node1:/home/ubuntu/cuda-samples/Samples/1\_Utilities/bandwidthTest# ./bandwidthTest

[CUDA Bandwidth Test] - Starting...

Running on...

Device 0: NVIDIA A100 80GB PCIe Quick Mode

Host to Device Bandwidth, 1 Device(s)

**PINNED Memory Transfers** 

Transfer Size (Bytes) Bandwidth(GB/s)

32000000 25.0

Device to Host Bandwidth, 1 Device(s)

PINNED Memory Transfers

Transfer Size (Bytes) Bandwidth(GB/s)

32000000 24.9

Device to Device Bandwidth, 1 Device(s)

**PINNED Memory Transfers** 

Transfer Size (Bytes) Bandwidth(GB/s)

32000000 549.7

Result = PASS

**Note:** The CUDA Samples are not meant for performance measurements. Results may vary when GPU Boost is enabled.

#### Install NVIDIA HPC SDK

#### Prerequisites

Step 1. Download NVIDIA HPC SDK software: https://developer.nvidia.com/hpc-sdk-downloads

\$ wget <u>https://developer.download.nvidia.com/hpc-</u> sdk/23.9/nvhpc 2023 239 Linux x86 64 cuda multi.tar.gz

\$ scp nvhpc\_2023\_239\_Linux\_x86\_64\_cuda\_multi.tar.gz ubuntu@10.29.148.171:/home/ubuntu/

Step 2. Copy NVIDIA HPC SDK to all nodes:

\$ ansible all -m copy -a "src=/home/ubuntu/nvhpc\_2023\_239\_Linux\_x86\_64\_cuda\_multi.tar.gz dest=/home/ubuntu/nvhpc\_2023\_239\_Linux\_x86\_64\_cuda\_multi.tar.gz"

\$ ansible all -m shell -a "tar xpzf /home/ubuntu/nvhpc\_2023\_239\_Linux\_x86\_64\_cuda\_multi.tar.gz"

Step 3. Install NVIDIA HPC SDK (optionally - select where it gets installed):

\$ ansible all -m shell -a "tar xpzf /home/ubuntu/nvhpc\_2023\_239\_Linux\_x86\_64\_cuda\_multi.tar.gz"

**Step 4.** Install NVIDIA HPC SDK:

\$ su - root

\$ cd nvhpc\_2023\_239\_Linux\_x86\_64\_cuda\_multi/

\$ sudo ./install

Step 5. Press Enter to continue installing NVIDIA HPC SDK:

**Step 6.** Select Install option:

An auto installation is appropriate for any scenario. The HPC SDK

configuration (localrc) is created at first use and stored in each user's

home directory.

Installation directory? [/opt/nvidia/hpc\_sdk]

- 1 Single system install
- 2 Network install
- 3 Auto install

Please choose install option:

3

Step 7. Select default directory or intended location:

Please specify the directory path under which the software will be installed.

The default directory is /opt/nvidia/hpc\_sdk, but you may install anywhere

you wish, assuming you have permission to do so.

Installation directory? [/opt/nvidia/hpc\_sdk]

#### Tech tip

Installing NVIDIA HPC SDK version 23.9 into /opt/nvidia/hpc\_sdk Making symbolic link in /opt/nvidia/hpc\_sdk/Linux\_x86\_64 generating environment modules for NV HPC SDK 23.9 ... done. Installation complete. HPC SDK successfully installed into /opt/nvidia/hpc\_sdk If you use the Environment Modules package, that is, the module load command, the NVIDIA HPC SDK includes a script to set up the appropriate module files. % module load /opt/nvidia/hpc\_sdk/modulefiles/nvhpc/23.9 % module load nvhpc/23.9 Alternatively, the shell environment may be initialized to use the HPC SDK. In csh, use these commands: % setenv MANPATH " \$MANPATH" :/opt/nvidia/hpc\_sdk/Linux\_x86\_64/23.9/compilers/man % set path = (/opt/nvidia/hpc\_sdk/Linux\_x86\_64/23.9/compilers/bin \$path) In bash, sh, or ksh, use these commands: \$ MANPATH=\$MANPATH:/opt/nvidia/hpc\_sdk/Linux\_x86\_64/23.9/compilers/man; export MANPATH \$ PATH=/opt/nvidia/hpc\_sdk/Linux\_x86\_64/23.9/compilers/bin:\$PATH; export PATH Once the 64-bit compilers are available, you can make the OpenMPI commands and man pages accessible using these commands. % set path = (/opt/nvidia/hpc\_sdk/Linux\_x86\_64/23.9/comm\_libs/mpi/bin \$path) % setenv MANPATH "\$MANPATH":/opt/nvidia/hpc\_sdk/Linux\_x86\_64/23.9/comm\_libs/mpi/man And the equivalent in bash, sh, and ksh: \$ export PATH=/opt/nvidia/hpc\_sdk/Linux\_x86\_64/23.9/comm\_libs/mpi/bin:\$PATH \$ export MANPATH=\$MANPATH:/opt/nvidia/hpc\_sdk/Linux\_x86\_64/23.9/comm\_libs/mpi/man

Please check https://developer.nvidia.com for documentation, use of NVIDIA HPC SDK software, and other questions.

Step 8. Install environement-modules:

\$ ansible all -m shell -a " sudo apt-get install -y environment-modules"

\$ cat /etc/profile.d/modules.sh

shell=\$(/usr/bin/basename \$(/bin/ps -p \$\$ -ocomm=))

if [ -f /usr/share/modules/init/\$shell ]; then

. /usr/share/modules/init/\$shell

#### else

. /usr/share/modules/init/sh

```
fi
```

Step 9. Create environment variables to be set at the time of user login:

\$ vi /etc/environment

# Use the HPC SDK toolkit compilers

export NVIDIA=/opt/hpc/nvidia/hpc\_sdk

module use \$NVIDIA/modulefiles

module load nvhpc

# But then override their choice of Open MPI to use the HPCX that is inside the HPC SDK

module use /opt/hpc/nvidia/hpc\_sdk/Linux\_x86\_64/2023/comm\_libs/12.2/hpcx/hpcx-2.15/modulefiles

module load hpcx

\$ source /etc/environment

\$printenv

Step 10. Verify above configured modules are loaded and "mpirun" and "mpicc" available:

\$ which mpirun

/opt/hpc/nvidia/hpc\_sdk/Linux\_x86\_64/23.7/comm\_libs/12.2/hpcx/hpcx-2.15/ompi/bin/mpirun

\$ which mpicc

/opt/hpc/nvidia/hpc\_sdk/Linux\_x86\_64/23.7/comm\_libs/12.2/hpcx/hpcx-2.15/ompi/bin/mpicc
## Solution Validation

This chapter contains the following:

What is GPUDirect?

## What is GPUDirect?

NVIDIA GPUDirect RDMA (Remote Direct Memory Access) is a technology that enables a direct path for data exchange between the GPU and third-party peer devices using standard PCIe features. GPUDirect RDMA relies on the ability of NVIDIA GPUs to expose portions of device memory in a PCIe base address register region, as shown in <u>Figure 12</u>. The GPUDirect technology requires a PCIe Switch to facilitate direct memory transfer between NVIDIA NIC and GPU.

A PCIe switch is not strictly required to enable GPUDirect RDMA on a supported system. Please refer to How GPUDirect RDMA works, NVIDIA GPUDirect Storage design guide, and <u>GPUDirect RDMA supported systems</u> for more details.

If there is no PCIe switch between network interface card and NVIDIA GPU, data has to traverse through processor. Performance improvement achieved through GPUDirect RDMA, and benefits depend on your use case and system configuration.



#### Figure 12. GPUDirect Vs No GPUDirect

**Note:** A requirement for GPUDirect RDMA to work is that the NVIDIA GPU and the Mellanox Adapter share the same root complex through a PCIe switch.

**Note:** For our solution, we could not use GPUDirect as Cisco UCS C240 M7 rack server does not contain PCIe switch between CPU and Mellanox Ethernet NIC and NVIDIA GPU as shown in <u>Figure 12</u>.

## **NVIDIA HPC-X Software Toolkit Setup and Configuration**

This section details the validation of the HPC/AI cluster previously configured.

- Prerequisites
- Test Result for NVIDIA HPC-X Software Toolkit
- NVIDIA HPC-X Software Toolkit Test Summary

#### **Prerequisites**

Test toolkit to validate the end-end connectivity.

**Note:** We installed NVIDIA HPC-X software toolkit version 2.16 for the validation.

For more details, go to: https://docs.nvidia.com/networking/display/hpcxv216

#### Tech tip

MPI (Message Passing Interface) is a standard and widely used library and protocol for writing parallel applications in HPC.

"mpirun" is a command used in HPC part of MPI implementation, such as OpenMPI and MPICH which provides the underlying libraries and runtime support for parallel programming. When combined with these MPI libraries, "mpirun" becomes a powerful tool for launching, managing, and scaling parallel applications in HPC environments, making it possible to harness the computational power of clusters and supercomputers for scientific simulations, data analysis, and other compute-intensive tasks.

"mpicc" streamlines the process of compiling parallel C and C++ programs for use in HPC environments, allowing developers to take full advantage of the parallel processing capabilities of these systems.

"mpich" is one of the primary implementations of the MPI standard. It provides a set of libraries, tools, and runtime environments that allow developers to create parallel applications in C, C++, and Fortran.

OpenACC (Open Accelerators) is an open standard for parallel programming of heterogeneous computer systems, including multi-core CPUs and GPUs (Graphics Processing Units). It provides a set of directives, libraries, and APIs that enable developers to accelerate their applications by offloading compute-intensive portions to accelerators, such as GPUs, while maintaining a single source code that can run on both CPUs and GPUs.

UCX (Unified Communication X) s an open-source communication library designed for high-performance computing (HPC) and other parallel computing environments. UCX is particularly valuable for applications that rely on efficient communication in HPC and parallel computing scenarios. It allows these applications to achieve high performance while maintaining portability across diverse hardware and networking environments.

Step 1. Accept EUL agreement to download NVIDIA HPC-X clusterkit:

\$ wget http://www.mellanox.com/page/hpcx\_eula?mrequest=downloads&mtype=hpc&mver=hpcx&mname=v2.16.2/hpcx-v2.16-qcc-mlnx\_ofed-ubuntu22.04-cuda12-qdrcopv2-nccl2.18-x86\_64.tbz

Step 2. Copy HPC-X software toolkit on all nodes:

\$ scp hpcx-v2.16-gcc-mlnx\_ofed-ubuntu22.04-cuda12-gdrcopy2-nccl2.18-x86\_64.tbz ubuntu@10.29.148.171:/home/ubuntu/

\$ ansible all -m copy -a "src=/home/ubuntu/hpcx-v2.16-gcc-mlnx\_ofed-ubuntu22.04-cuda12-gdrcopy2nccl2.18-x86\_64.tbz dest=/home/ubuntu/hpcx-v2.16-gcc-mlnx\_ofed-ubuntu22.04-cuda12-gdrcopy2nccl2.18-x86\_64.tbz"

**Step 3.** Extract HPC-X software toolkit:

\$ ansible all -m shell -a "tar -xvf /home/ubuntu/hpcx-v2.16-gcc-mlnx\_ofed-ubuntu22.04-cuda12-gdrcopy2nccl2.18-x86\_64.tbz"

Step 4. Update shell variable of the location of HPC-X installation:

\$ cd /home/ubuntu/hpcx-v2.16-gcc-mlnx\_ofed-ubuntu22.04-cuda12-gdrcopy2-nccl2.18-x86\_64

\$ export HPCX\_HOME=\$PWD

**Step 5.** Build and Run applications with HPC-X. To load OpenMPI based package run following commands:

\$ source \$HPCX\_HOME/hpcx-init.sh

\$ hpcx\_load

\$ env | grep HPCX

\$ mpicc \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_c.c -o \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_c

\$ mpirun -np 2 \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_c

Hello, world, I am 0 of 2, (Open MPI v4.1.5rc2, package: Open MPI root@hpc-kernel-03 Distribution, ident: 4.1.5rc2, repo rev: v4.1.5rc1-17-gdb10576f40, Unreleased developer copy, 150)

Hello, world, I am 1 of 2, (Open MPI v4.1.5rc2, package: Open MPI root@hpc-kernel-03 Distribution, ident: 4.1.5rc2, repo rev: v4.1.5rc1-17-gdb10576f40, Unreleased developer copy, 150)

\$ oshcc \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_oshmem\_c.c -o \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_oshmem\_c

\$ oshrun -np 2 \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_oshmem\_c

Hello, world, I am 1 of 2: http://www.open-mpi.org/ (version: 1.4)

Hello, world, I am 0 of 2: http://www.open-mpi.org/ (version: 1.4)

\$ hpcx\_unload

Step 6. Run following command: (optional) If not installed already; install environment-modules:

\$ ansible all -m shell -a "sudo apt install environment-modules -y"

\$ ansible all -m shell -a "source ~/.bashrc"

\$ ansible all -m shell -a "source ~/.profile"

\$ ansible all -m shell -a "sudo modprobe knem"

**Step 7.** Building HPC-X with Intel Compiler Suite:

**Note:** As of version 1.7, HPC-X builds are no longer distributed based on the Intel compiler suite. However, after following the HPC-X deployment example below, HPC-X can subsequently be rebuilt from source with your Intel compiler suite as follows:

\$ tar xfp \${HPCX\_HOME}/sources/openmpi-gitclone.tar.gz

\$ cd \${HPCX\_HOME}/sources/openmpi-gitclone

\$ Is -I \${HPCX\_HOME}/sources/openmpi-gitclone.tar.gz

-rw-r--r-- 1 ubuntu ubuntu 18287983 Aug 3 13:59 /home/ubuntu/hpcx-v2.16-gcc-mlnx\_ofed-ubuntu22.04cuda12-gdrcopy2-nccl2.18-x86\_64//sources/openmpi-gitclone.tar.gz

\$ cd \${HPCX\_HOME}/sources/openmpi-gitclone

\$ ./configure CC=icx CXX=icpx F77=ifort FC=ifort --prefix=\${HPCX\_HOME}/ompi-icc \

--with-hcoll=\${HPCX\_HOME}/hcoll \

--with-ucx=\${HPCX\_HOME}/ucx \

--with-platform=contrib/platform/mellanox/optimized \

2>&1 | tee config-icc-output.log

\$ make -j32 all 2>&1 | tee build\_icc.log && make -j24 install 2>&1 | tee install\_icc.log

**Step 8.** Load HPC-X environment from modules:

\$ module use \$HPCX\_HOME/modulefiles

\$ module load hpcx

\$ mpicc \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_c.c -o \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_c

\$ mpirun -np 2 \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_c

Hello, world, I am 1 of 2, (Open MPI v4.1.5rc2, package: Open MPI root@hpc-kernel-03 Distribution, ident: 4.1.5rc2, repo rev: v4.1.5rc1-17-gdb10576f40, Unreleased developer copy, 150)

Hello, world, I am 0 of 2, (Open MPI v4.1.5rc2, package: Open MPI root@hpc-kernel-03 Distribution, ident: 4.1.5rc2, repo rev: v4.1.5rc1-17-gdb10576f40, Unreleased developer copy, 150)

\$ oshcc \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_oshmem\_c.c -o \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_oshmem\_c

\$ oshrun -np 2 \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_oshmem\_c

Hello, world, I am 1 of 2: http://www.open-mpi.org/ (version: 1.4)

Hello, world, I am 0 of 2: http://www.open-mpi.org/ (version: 1.4)

**Step 9.** To profile MPI API run following command: (Optional)

\$ export IPM\_KEYFILE=\$HPCX\_IPM\_DIR/etc/ipm\_key\_mpi

\$ export IPM\_LOG=FULL

\$ export LD\_PRELOAD=\$HPCX\_IPM\_DIR/lib/libipm.so

\$ \$HPCX\_IPM\_DIR/bin/ipm\_parse -html outfile.xml

\$ export IPM\_ADD\_BARRIER\_TO\_REDUCE=1

\$ export IPM\_ADD\_BARRIER\_TO\_ALLREDUCE=1

\$ export IPM\_ADD\_BARRIER\_TO\_GATHER=1

\$ export IPM\_ADD\_BARRIER\_TO\_ALL\_GATHER=1

\$ export IPM\_ADD\_BARRIER\_TO\_ALLTOALL=1

\$ export IPM\_ADD\_BARRIER\_TO\_ALLTOALLV=1

\$ export IPM\_ADD\_BARRIER\_TO\_BROADCAST=1

\$ export IPM\_ADD\_BARRIER\_TO\_SCATTER=1

\$ export IPM\_ADD\_BARRIER\_TO\_SCATTERV=1

\$ export IPM\_ADD\_BARRIER\_TO\_GATHERV=1

\$ export IPM\_ADD\_BARRIER\_TO\_ALLGATHERV=1

\$ export IPM\_ADD\_BARRIER\_TO\_REDUCE\_SCATTER=1

**Step 10.** Create hotfile.txt in /home/ubuntu/hpcx-v2.16-gcc-mlnx\_ofed-ubuntu22.04-cuda12-gdrcopy2-nccl2.18-x86\_64/clusterkit/bin/

\$ vi hostfile.txt

hpc-node1

hpc-node2

hpc-node3

••••

hpc-node8

**Step 11.** UCX intra-node communication uses the KNEM module, which improves the performance significantly. Make sure this module is loaded on your system:

\$ modprobe knem

**Step 12.** When HPC-X is launched with Open MPI without a resource manager job environment (slurm,pbs, and so on), or when it is launched from a compute node, the default rsh/ssh-based launcher will be used. This launcher does not propagate environment variables to the compute nodes. Thus, it is important to ensure the propagation of LD\_LIBRARY\_PATH variable from HPC-x is done as follows:

\$ mpirun -x LD\_LIBRARY\_PATH -np 2 -H hpc-node1,hpc-node2,hpc-node3,hpc-node4 \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_c

Sample Command:

\$ mpirun -x LD\_LIBRARY\_PATH -np 2 -H host1,host2 \$HPCX\_MPI\_TESTS\_DIR/examples/hello\_c

**Step 13.** After loading HPC-X package; run clusterkit script or using the "mpirun" command:

# mpirun

\$ mpirun -x LD\_LIBRARY\_PATH -np 2 -H c240m7-13,c240m7-14 \$HPCX\_CLUSTERKIT\_DIR/bin/clusterkit

Note: ClusterKit runs by default in pairwise test cases, which requires at least two nodes to run.

# clusterkit script

**Note:** \$ ./clusterkit.sh -h for list of options and parameters.

#### Test Results for NVIDIA HPC-X Software Toolkit

Clusterkit part of the NVIDIA HPC-X software toolkit is a multifaceted node assessment tool for high performance clusters. Currently, ClusterKit is capable of testing latency, bandwidth, effective bandwidth, memory bandwidth, GFLOPS by node, per-rack collective performance, as well as bandwidth and latency between GPUs and local/remote memory. ClusterKit employs well known techniques and tests to arrive at these performance metrics and is intended to give the user a general look at the health and performance of a cluster.

**Step 1.** A sample command ran to measure performance and HPC/AI cluster configuration for this solution test and validate:

\$ ./clusterkit.sh --ssh --hostfile hostfile.txt -y --hca\_list "mlx5\_0:1,mlx5\_1:1" -z 15

**Note:** mlx5\_0 and mlx5\_1 are two physical ports on ConnectX6-DX ethernet NIC installed on each Cisco UCS C240 M7 Rack Server

**Step 2.** Test result generated by HPC-X Clusterkit command which runs for 15 minute interval can be found here:

~/hpcx-v2.16-gcc-mlnx\_ofed-ubuntu22.04-cuda12-gdrcopy2-nccl2.18x86\_64/clusterkit/bin/20231103\_134557\$ cat bandwidth.txt Cluster: Unknown User: ubuntu Testname: bandwidth Date\_and\_Time: 2023/11/03 13:45:58 JOBID: 0 PPN: 128 **Bidirectional: True** Skip\_Intra\_Node: True HCA\_Tag: Unknown Technology: Unknown Bandwidth\_bidir (MB/s): Message size: 8388608 B Iterations: 10000 Rank: 0 1 2 3 4 5 7 6 0 (hpc-node1): 0.0 48829.3 48381.3 48377.6 48823.9 48840.8 48839.7 48842.8 1 (hpc-node2): 48829.3 0.0 48393.2 48372.8 48841.4 48853.4 48856.3 48853.9 2 (hpc-node3): 48381.3 48393.2 0.0 48347.1 48396.5 48387.9 48389.8 48382.1 3 (hpc-node4): 48377.6 48372.8 48347.1 0.0 48369.2 48378.3 48367.7 48374.7 4 (hpc-node5): 48823.9 48841.4 48396.5 48369.2 0.0 48839.0 48842.8 48839.5 5 (hpc-node6): 48840.8 48853.4 48387.9 48378.3 48839.0 0.0 48857.7 48865.4 6 (hpc-node7): 48839.7 48856.3 48389.8 48367.7 48842.8 48857.7 0.0 48859.3 7 (hpc-node8): 48842.8 48853.9 48382.1 48374.7 48839.5 48865.4 48859.3 0.0 Minimum bandwidth: 48347.1 MB/s between hpc-node3 and hpc-node4 Maximum bandwidth: 48865.4 MB/s between hpc-node6 and hpc-node8 Average bandwidth: 48628.7 MB/s

#### NVIDIA HPC-X Software Toolkit Test Summary

When running NVIDIA HPC-X Software toolkit based Clusterkit test; we observed ~200Gbps bandwidth is achieved (Duplex on two 100Gbps port; mlx5\_0 and mlx5\_1 are two physical ports on ConnectX6-DX ethernet NIC installed on each Cisco UCS C240 M7 Rack Server) when measuring host connectivity bandwidth between Cisco UCS C240 M7 server and a pair of Cisco Nexus 93600CD-GX leaf switch.

The following screenshot shows line-rate network traffic generated when running NVIDIA HPC-X Clusterkit command above to measure network bandwidth for longer duration. Line-rate traffic was monitored between

Cisco UCS C240 M7 with Mellanox ConnectX-6 ethernet NIC ports connected to a pair of Cisco Nexus 93600CD-GX leaf switch.

Figure 13. Screenshot monitoring port utilization on Cisco Nexus 93600CD-GX leaf1(A) and leaf2(B) connected to Cisco UCS C240 M7 Rack Server with 2 x 100GbE Mellanox ConnectX6 Ethernet NIC

very 2.0s		vsh		sh in	t	sjc2-	g18-lea	f1: F	ri Nov	3 13	:59:1	6 2023	Every 2.	0s:	vs	h-c	"sh i	nt	sjc2-	g18-lea	f2: F	ri Nov	3 13	:59:1	6 2023
input	rat	e 98	.39	Gbps,	2.96	Mpps;	output	rate	98.39	Gbps,	2.96	6 Mpps	inpu	t n	ate	98.44	4 Gbps	, 2.97	Mpps;	output	rate	98.44	Gbps,	2.97	Mpps
input	rate	e 98	.29	Gbps,	2.95	Mpps;	output	rate	98.29	Gbps,	2.95	6 Mpps	inpu	t r	ate	98.30	) Gbps	, 2.96	Mpps;	output	rate	98.30	Gbps,	2.96	Mpps
input	rat	e 98	1.38	Gbps,	2.96	Mpps;	output	rate	98.38	Gbps,	2.96	i Mpps	inpu	t r	ate	98.42	2 Gbps	, 2.97	Mpps;	output	rate	98.42	Gbps,	2.97	Mpps
input	rat	e 98	1.24	Gbps,	2.95	Mpps;	output	rate	98.24	Gbps,	2.95	Mpps	inpu	t r	ate	98.23	3 Gbps	, 2.96	Mpps;	output	rate	98.22	Gbps,	2.96	Mpps
input	rat	e 98	1.29	Gbps,	2.95	Mpps;	output	rate	98.29	Gbps,	2.95	i Mpps	inpu	t r	ate	98.30	Gbps	, 2.96	Mpps;	output	rate	98.30	Gbps,	2.96	Mpps
input	rat	e 98	.28	Gbps,	2.95	Mpps;	output	rate	98.28	Gbps,	2.95	i Mpps	inpu	t n	ate	98.29	Gbps	, 2.96	Mpps;	output	rate	98.29	Gbps,	2.96	Mpps
input	rate	e 98	.29	Gbps,	2.95	Mpps;	output	rate	98.29	Gbps,	2.95	6 Mpps	inpu	t n	ate	98.30	) Gbps	, 2.96	Mpps;	output	rate	98.30	Gbps,	2.96	Mpps
input	rate	e 98	.28	Gbps,	2.95	Mpps;	output	rate	98.28	Gbps,	2.95	6 Mpps	inpu	t n	ate	98.29	9 Gbps	, 2.96	Mpps;	output	rate	98.29	Gbps,	2.96	Mpps
input	rat	e 98	1.14	Gbps,	2.95	Mpps;	output	rate	98.14	Gbps,	2.95	6 Mpps	inpu	t r	ate	98.13	3 Gbps	, 2.96	Mpps;	output	rate	98.13	Gbps,	2.96	Mpps
input	rat	e 98	1.28	Gbps,	2.95	Mpps;	output	rate	98.28	Gbps,	2.95	Mpps	inpu	t n	ate	98.28	3 Gbps	, 2.96	Mpps;	output	rate	98.28	Gbps,	2.96	Mpps
input	rat	e 98	.14	Gbps,	2.95	Mpps;	output	rate	98.14	Gbps,	2.95	i Mpps	inpu	t r	ate	98.12	2 Gbps	, 2.96	Mpps;	output	rate	98.12	Gbps,	2.96	Mpps
input	rat	e 98	.28	Gbps,	2.95	Mpps;	output	rate	98.28	Gbps,	2.95	i Mpps	inpu	t n	ate	98.28	3 Gbps	, 2.96	Mpps;	output	rate	98.28	Gbps,	2.96	Mpps
input	rat	e 98	.30	Gbps,	2.95	Mpps;	output	rate	98.30	Gbps,	2.95	Mpps	inpu	t r	ate	98.35	5 Gbps	, 2.96	Mpps;	output	rate	98.35	Gbps,	2.96	Mpps
input	rat	e 98	1.29	Gbps,	2.95	Mpps;	output	rate	98.29	Gbps,	2.95	6 Mpps	inpu	t n	ate	98.36	) Gbps	, 2.96	Mpps;	output	rate	98.30	Gbps,	2.96	Mpps
input	rat	e 98	1.31	Gbps,	2.95	Mpps;	output	rate	98.31	Gbps,	2.95	6 Mpps	inpu	t r	ate	98.36	6 Gbps	, 2.96	Mpps;	output	rate	98.36	Gbps,	2.96	Mpps
input	rat	e 98	.33	Gbps,	2.95	Mpps;	output	rate	98.33	Gbps,	2.95	6 Mpps	inpu	t r	ate	98.36	5 Gbps	, 2.96	Mpps;	output	rate	98.36	Gbps,	2.96	Mpps

Figure 14. Grafana dashboard monitoring ingress and egress network bandwidth on Cisco Nexus 93600CD-GX leaf 1



#### Test

This section highlights test result for the datasets of different size and application area. Tests were executed to determine cluster scalability, clock time required to complete each said dataset on CPU only and repeat the same on a system with one or two GPU per system.

CPU only tests were executed with all logical cores utilized on each node via adding parameter -np 128\*x (x= multiplier representative of number of nodes utilized).

We captured system performance statistics such as CPU utilization (vmstat), GPU utilization (nvidia-smi and NVIDIA GPU exporter Grafana WebUI console) and Network port utilization on Cisco Nexus switch connected to Cisco UCS server and NetApp A400 Storage when running the same test in a clustered configuration.

We tested combination of one, two, four and eight nodes to showcase linear scalability of the solution.

Test result shows clock time in second to complete each test scenario whether running on CPU or GPU.

#### **HPC Workload Dataset**

#### Prerequisites

We tested documented solution with HPC datasets representing different area/applications list below:

**Note:** Workload listed is for the proof of concept (PoC) purpose only.

#### 1. The MiniWeather Mini App (Weather)

The miniWeather code mimics the basic dynamics seen in atmospheric weather and climate. The dynamics themselves are dry compressible, stratified, non-hydrostatic flows dominated by buoyant forces that are relatively small perturbations on a hydrostatic background state. The equations in this code themselves form the backbone of pretty much all fluid dynamics codes, and this particular flavor forms the base of all weather and climate modeling.

For more details: https://github.com/mrnorman/miniWeather#openacc-accelerator-threading

#### 2. Minisweep (Nuclear Engineering)

Minisweep is a deterministic Sn radiation transport miniapp used for performance optimization and performance model evaluation on HPC architectures.

For more details: https://github.com/wdj/minisweep

#### 3. HPGMG: High-performance Geometric Multigrid (Cosmology/Astrophysics)

HPGMG implements full multigrid (FMG) algorithms using finite-volume and finite-element methods. Different algorithmic variants adjust the arithmetic intensity and architectural properties that are tested. These FMG methods converge up to discretization error in one F-cycle, thus may be considered direct solvers. An F-cycle visits the finest level a total of two times, the first coarsening (8x smaller) 4 times, the second coarsening 6 times, etc.

For more details: <u>https://bitbucket.org/hpgmg/hpgmg/src/master/</u>

Fech tip									
Run the following command to find all the parameter.									
\$mpicc -help									
Subset is pasted below from "mpicchelp" for reference:									
Target-specific switches:									
-acc[=gpu host multicore [no]autopar [no]routineseq legacy strict verystrict sync [no]wait]									
Enable OpenACC directives									
gpu OpenACC directives are compiled for GPU execution only; please refer to -gpu for target specific options									
host Compile for serial execution on the host CPU									
multicore Compile for parallel execution on the host CPU									
[no]autopar Enable (default) or disable loop autoparallelization within acc parallel									
[no]routineseq Compile every routine for the device									
legacy Suppress warnings about deprecated PGI accelerator directives									

strict	Issue warnings for non-OpenACC accelerator directives
verystrict	Fail with an error for any non-OpenACC accelerator directive
sync	Ignore async clauses
[no]wait	Wait for each device kernel to finish

The workload dataset tested in this solution to create a baseline has minimum system requirement based on the application and dataset size. Intention is to target varied cluster sizes with node count, core count and GPU count and their relative impact when running benchmark application to determined overall cluster performance.

- The Small size dataset target a single larger node or a small cluster of nodes using between 64 and 1024 ranks. It uses a maximum of 480GB of memory per benchmark.
- The Medium size dataset target a mid-sized cluster of nodes using between 256 and 4096 ranks. It uses a maximum of 4TB of memory per benchmark.
- The Large size dataset target a larger cluster of nodes using between 2048 and 32,768 ranks. It uses a maximum of 14.5TB of memory per benchmark.

For this solution, datasets were downloaded and configured in the shared NFS volume on NetApp A400 storage and used NetApp FlexClone volumes to mount on each node part of the HPC cluster test. We tested following possible combinations for scale tests on HPC cluster workloads.

Scale Test	1-node	2-node	4-node	8-node
C240M7 Server with 1x A100 GPU				
C240M7 Server with 2x A100 GPU				
C240M7 Server with CPU only				

 Table 6.
 Configuration tested for scale tests

**Note:** We will extend this exercise with 8 node HPC cluster with 2 x NVIDIA Tesla A100-80G GPU per node in the future.

## Application 1: miniWeather (Large Size Dataset)

Table 7 lists the results from scale out tests on miniWeather.

Table 7. Scale test results with miniWeather large size dataset in se	cond
---	------

Scale Test	1-node (Total time in second)	2-node (Total time in second)	4-node (Total time in second)	8-node (Total time in second)
C240M7 Server with 1x A100 GPU	1048.16	518.98	246.16	109.27
C240M7 Server with 2x A100 GPU	518.34	245.61	105.85	NA
C240M7 Server with CPU only	3418.28	1726.53	865.28	436.14



Figure 15. Cluster scalability when running Large miniWeather Dataset



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Figure 17. % Avg GPU utilization when running Large miniWeather Dataset on nodes w/ 1 NVIDIA A100-80G GPU





Figure 18. % Avg GPU utilization when running Large miniWeather Dataset on nodes w/ 2 NVIDIA A100-80G GPU







Figure 20. % Avg GPU memory utilization when running Large miniWeather Dataset on nodes w/ 2 NVIDIA A100-80G GPU





Figure 22. Sample % Avg network utilization when running Large miniWeather Dataset on 8 node w/ 1 x A100-80G GPU per node

Eve	ry 2.0	s: v	sh -c	"sh i.	s	jc2-g1	8-leaf2	: Thu	Nov	9 12:2	4:42	2023	Ev	ery 2.0	5: V	sh -c	"sh i.	5	jc2-g1	8-leaf1	: Thu	Nov	9 12:2	4:42	2023
0-01	input	rate	67.71	Mbps,	3.52	Kpps;	output	rate	67.71	Mbps,	3.52	Крр		input	rate	68.28	Mbps,	2.28	Kpps;	output	rate	68.28	8 Mbps,	2.28	Крр
5	input	rate	33.95	Mbps,	1 <mark>.</mark> 73	Kpps;	output	rate	34.63	Mbps,	1.73	в Крр	5	input	rate	34.04	Mbps,	1.10	Kpps;	output	rate	34.04	Mbps,	1.10	Крр
s	input	rate	67.71	Mbps,	3.52	Kpps;	output	rate	67.71	Mbps,	3.52	Крр	s	input	rate	68.27	Mbps,	2.28	Kpps;	output	rate	68.27	Mbps,	2.28	Крр
5	input	rate	33.94	Mbps,	1.73	Kpps;	output	rate	34.61	Mbps,	1.73	Крр	5	input	rate	34.50	Mbps,	1.11	Kpps;	output	rate	34.50	) Mbps,	1.11	Крр
s	input	rate	67.71	Mbps,	3.52	Kpps;	output	rate	67.71	Mbps,	3.52	Kpp	s	input	rate	68.26	Mbps,	2.28	Kpps;	output	rate	68.26	5 Mbps,	2.28	Крр
s	input	rate	33.94	Mbps,	1.73	Kpps;	output	rate	34.61	Mbps,	1.73	Крр	s	input	rate	34.50	Mbps,	1.11	Kpps;	output	rate	34.50	) Mbps,	1.11	Крр
s	input	rate	67.71	Mbps,	3.52	Kpps;	output	rate	67.71	Mbps,	3.52	Kpp	s	input	rate	68.26	Mbps,	2.28	Kpps;	output	rate	68.26	5 Mbps,	2.28	Крр
s	input	rate	33.94	Mbps,	1.73	Kpps;	output	rate	34.61	Mbps,	1.73	Крр	s	input	rate	34.50	Mbps,	1.11	Kpps;	output	rate	34.50	) Mbps,	1.11	Крр
s	input	rate	67.71	Mbps,	3.52	Kpps;	output	rate	67.71	Mbps,	3.52	Kpp	s	input	rate	68.26	Mbps,	2.28	Kpps;	output	rate	68.26	5 Mbps,	2.28	Крр
s	input	rate	33.93	Mbps,	1.73	Kpps;	output	rate	33.93	Mbps,	1.73	Крр	s	input	rate	34.51	Mbps,	1.11	Kpps;	output	rate	35.17	Mbps,	1.11	Крр
s	input	rate	67.71	Mbps.	3.52	Kpps:	output	rate	67.71	Mbps.	3.52	Kpp	s	input	rate	68.26	Mbps.	2.28	Kpps:	output	rate	68.26	5 Mbps.	2.28	Крр
s	input	rate	33.93	Mbps.	11.73	Kops:	output	rate	33.93	Mbps.	1.73	Kpp	s	input	rate	34.51	Mbps.	1.11	Kpps:	output	rate	35.17	Mbps.	1.11	Kpp
s	input	rate	67.71	Mbps.	3.52	Kons:	output	rate	67.71	Mbps.	3.52	Knn	s	input	rate	68.27	Mbps.	2.28	Kons:	output	rate	68.27	Mbps.	2.28	Knn
s	input	rate	33 93	Mbns	1 73	Kons:	output	rate	33 93	Mhns	1 73	Kon	s	input	rate	34 51	Mbps,	1 11	Kons:	output	rate	35 17	Mbps,	1 11	Knn
s	input	rate	67 71	Mbps,	2 52	Konce	output	rate	67 71	Mbpc	3 53	Kpp	s	input	rate	69.37	Mbpc	2 20	Kons.	output	rate	69 27	Mbps,	2 29	Kpp
s	input	Tate	22.02	mops,	3.52	Kpps;	output	rate	07.71	mops,	3.52	Крр	s	unput	Tate	00.2/	mops,	2.28	Kpps;	output	Tate	00.27	ribps,	2.28	крр
s	input	rate	33.93	mops,	1.73	кррs;	output	rate	33.93	mops,	1./3	крр	s	input	rate	34.51	mops,	1.11	kpps;	output	rate	35.18	s mops,	1.11	крр

#### **Observations**

Figure 23. 8 Node HPC Cluster comparison with miniWeather larger dataset test on 1 x NVIDIA A100-80G GPU vs Dual Socket CPU





The following observations were made from the test results obtained by running miniWeather large dataset on the 8 x Cisco UCS C240 M7 node based HPC cluster as defined in this solution study:

- The end-end FlexPod HPC cluster as highlighted in this solution scaled linearly whether the cluster test ran by CPU only or w/ GPU.
- Each node resources i.e., compute, storage and network consumed evenly throughout the cluster test.
- 100% GPU utilization and memory utilization.
- No CPU cycles were consumed when ran the test on NVIDIA A100-80G GPU.
- Time to complete the test with one GPU per node in an eight-node cluster is 4x faster than running the same test on eight-node cluster without GPU.

#### Application 2: Minisweep (Small Size Dataset)

Table 8 lists the results from scale out tests on Minisweep.

#### Table 8. Scale test results with Minisweep small size dataset in second

Scale Test	1-node (Total time in second)	2-node (Total time in second)	4-node (Total time in second)	8-node (Total time in second)		
C240M7 Server with 1x A100 GPU	438.10	217.18	122.93	76.21		
C240M7 Server with 2x A100 GPU	216.99	130.58	87.10	NA		
C240M7 Server with CPU only	1927.84	1045.48	742.04	435.59		



Figure 24. Cluster scalability when running small miniSweep Dataset.



Figure 25. % Avg CPU utilization when running Small miniSweep Dataset only on CPU



Figure 26. % Avg GPU utilization when running small Minisweep Dataset on nodes w/ 1 NVIDIA A100-80G GPU % Avg GPU Utilization for small Mnisweep Dataset running on 1 x NVIDIA A100-80G GPU per node

Figure 27. % Avg GPU utilization when running small Minisweep Dataset on nodes w/ 2 NVIDIA A100-80G GPU % Avg GPU Utilization for small Mnisweep Dataset running on 2 x NVIDIA A100-80G GPU per node





#### Figure 28. % Avg GPU memory utilization when running small Minisweep Dataset on nodes w/ 1 NVIDIA A100-80G GPU

Figure 29. % Avg GPU memory utilization when running small Minisweep Dataset on nodes w/ 2 NVIDIA A100-80G GPU



% Avg GPU memory Utilization for small Mnisweep Dataset running on 2 x NVIDIA A100-80G GPU per node

Figure 30. Sample % Avg network utilization when running small Minisweep Dataset on 8 node w/ 1 x A100-80G GPU per node

Every 2.0s: vsh -c "sh int eth sjc2-g18-leaf1: Tue Nov 7 15:43:06 2023	<sup>^</sup> Every 2.0s: vsh -c "sh int eth1/3-1 sjc2-g18-leaf2: Tue Nov 7 15:43:07 2023
input rate 1.75 Gbps, 53.34 Kpps; output rate 1.53 Gbps, 46.78 Kpps input rate 1.19 Gbps, 36.23 Kpps; output rate 1.16 Gbps, 35.52 Kpps input rate 3.30 Gbps, 101.02 Kpps; output rate 3.33 Gbps, 101.93 Kpps input rate 2.35 Gbps, 71.80 Kpps; output rate 2.35 Gbps, 71.94 Kpps input rate 2.35 Gbps, 72.01 Kpps; output rate 3.42 Gbps, 104.61 Kpps input rate 2.36 Gbps, 72.01 Kpps; output rate 3.47 Gbps, 104.67 Kpps input rate 3.38 Gbps, 103.50 Kpps; output rate 3.47 Gbps, 104.67 Kpps input rate 2.38 Gbps, 72.49 Kpps; output rate 3.47 Gbps, 72.07 Kpps input rate 2.38 Gbps, 103.50 Kpps; output rate 3.48 Gbps, 106.33 Kpps input rate 3.38 Gbps, 103.50 Kpps; output rate 3.47 Gbps, 72.07 Kpps input rate 3.38 Gbps, 102.39 Kpps; output rate 3.48 Gbps, 106.33 Kpps input rate 3.36 Gbps, 72.38 Kpps; output rate 3.48 Gbps, 72.77 Kpps input rate 3.36 Gbps, 102.90 Kpps; output rate 3.42 Gbps, 104.62 Kpps input rate 3.36 Gbps, 72.50 Kpps; output rate 3.33 Gbps, 72.77 Kpps input rate 3.31 Gbps, 72.50 Kpps; output rate 3.33 Gbps, 101.74 Kpps input rate 2.35 Gbps, 71.90 Kpps; output rate 3.36 Gbps, 71.94 Kpps input rate 2.35 Gbps, 53.15 Kpps; output rate 1.53 Gbps, 45.86 Kpps input rate 1.19 Gbps, 53.15 Kpps; output rate 1.16 Gbps, 35.55 Kpps	<pre>input rate 1.51 Gbps, 47.87 Kpps; output rate 1.70 Gbps, 53.45 Kpps input rate 1.18 Gbps, 38.24 Kpps; output rate 1.17 Gbps, 38.01 Kpps input rate 3.30 Gbps, 103.87 Kpps; output rate 3.27 Gbps, 102.93 Kpps input rate 2.36 Gbps, 75.29 Kpps; output rate 3.37 Gbps, 102.93 Kpps input rate 2.38 Gbps, 75.97 Kpps; output rate 2.37 Gbps, 75.44 Kpps input rate 2.38 Gbps, 75.87 Kpps; output rate 2.37 Gbps, 75.66 Kpps input rate 2.38 Gbps, 75.87 Kpps; output rate 2.37 Gbps, 79.66 Kpps input rate 2.40 Gbps, 76.65 Kpps; output rate 2.38 Gbps, 75.18 Kpps input rate 2.40 Gbps, 76.52 Kpps; output rate 2.38 Gbps, 76.18 Kpps input rate 2.40 Gbps, 76.52 Kpps; output rate 2.38 Gbps, 76.18 Kpps input rate 3.46 Gbps, 111.89 Kpps; output rate 3.47 Gbps, 109.43 Kpps input rate 2.39 Gbps, 76.31 Kpps; output rate 3.37 Gbps, 109.43 Kpps input rate 3.48 Gbps, 109.46 Kpps; output rate 3.37 Gbps, 106.16 Kpps input rate 3.32 Gbps, 76.27 Kpps; output rate 3.37 Gbps, 106.4 Kpps input rate 3.38 Gbps, 75.42 Kpps; output rate 3.37 Gbps, 55.3 Kpps input rate 3.38 Gbps, 75.42 Kpps; output rate 3.37 Gbps, 75.72 Kpps input rate 3.39 Gbps, 75.41 Kpps; output rate 3.37 Gbps, 75.73 Kpps input rate 3.36 Gbps, 75.41 Kpps; output rate 3.36 Gbps, 75.35 Kpps input rate 1.51 Gbps, 47.80 Kpps; output rate 1.72 Gbps, 54.04 Kpps input rate 1.18 Gbps, 38.19 Kpps; output rate 1.17 Gbps, 38.03 Kpps</pre>

#### Figure 31. Sample Grafana dashboard showing GPU statistics



#### **Observations**

Figure 32. 8 Node HPC Cluster comparison with Minisweep small dataset test on 1 x NVIDIA A100-80G GPU vs Dual Socket CPU







The following observations were made from the test results obtained by running Minisweep small dataset on the 8 x Cisco UCS C240 M7 node based HPC cluster as defined in this solution study:

- The end-end FlexPod HPC cluster as highlighted in this solution scaled linearly whether the cluster test ran by CPU only or w/ GPU.
- Each node resources i.e., compute, storage and network consumed evenly throughout the cluster test.
- Different than weather simulation exercise above the Nuclear Engineering Radiation Transport based Minisweep small dataset showed difference in overall GPU utilization; while we saw at the full cluster test approximately 90% GPU utilization and 70% memory utilization.
- No CPU cycles were consumed when ran the test on NVIDIA A100-80G GPU.
- Time to complete the test with one GPU per node in an eight-node cluster is 5.7x faster than running the same test on eight-node cluster without GPU.

#### Application 3: HPGMG (Medium Size Dataset)

Table 9 lists the results from scale out tests on HPGMG.

Scale Test	1-node (Total time in second)	2-node (Total time in second)	4-node (Total time in second)	8-node (Total time in second)		
C240M7 Server with 1x A100 GPU	NA	NA	308.76	190.16		
C240M7 Server with 2x A100 GPU	NA	305.33	182.86	NA		
C240M7 Server with CPU only	4524.42	2330.06	1229.69563	677.1356146		

#### Table 9. Scale test results with HPGMG medium size dataset in second.

Figure 33. Cluster scalability when running medium HPGMG Dataset





#### Figure 34. % Avg CPU utilization when running Medium HPGMG Dataset only on CPU



Figure 35. % Avg GPU utilization when running medium HPGMG Dataset on nodes w/ 1 NVIDIA A100-80G GPU







## Figure 37. % Avg GPU memory utilization when running medium HPGMG Dataset on nodes w/ 1 NVIDIA A100-80G GPU

Figure 38. % Avg GPU memory utilization when running medium HPGMG Dataset on nodes w/ 2 NVIDIA A100-80G GPU



% Avg GPU memory Utilization for HPGMG medioum Dataset running on 2 x NVIDIA A100-80G GPU per node

Figure 39. Sample % Avg network utilization when running medium HPGMG Dataset on 8 node w/ 1 x A100-80G GPU per node

Every 2.0s: vsh -c "sh int eth sjc2-g18-leaf1: Mon Nov 6 22:27:23 2023	<sup>^</sup> Every 2.0s: vsh -c "sh int eth1/3-1 sjc2-g18-leaf2: Mon Nov 6 22:27:23 2023
input rate 968.99 Mbps, 49.32 Kpps; output rate 968.88 Mbps, 49.23 Kpps input rate 970.94 Mbps, 49.42 Kpps; output rate 970.86 Mbps, 49.31 Kpps input rate 970.81 Mbps, 49.26 Kpps; output rate 970.86 Mbps, 49.25 Kpps input rate 970.81 Mbps, 49.26 Kpps; output rate 970.89 Mbps, 49.25 Kpps input rate 960.04 Mbps, 49.24 Kpps; output rate 970.89 Mbps, 49.32 Kpps input rate 970.86 Mbps, 49.24 Kpps; output rate 970.80 Mbps, 49.32 Kpps input rate 970.88 Mbps, 49.27 Kpps; output rate 970.86 Mbps, 49.32 Kpps input rate 968.98 Mbps, 49.35 Kpps; output rate 968.96 Mbps, 49.32 Kpps input rate 970.88 Mbps, 49.35 Kpps; output rate 970.86 Mbps, 49.32 Kpps	input rate 1.15 Gbps, 236.47 Kpps; output rate 1.15 Gbps, 236.57 Kpps input rate 1.15 Gbps, 236.98 Kpps; output rate 1.15 Gbps, 237.08 Kpps input rate 1.15 Gbps, 236.36 Kpps; output rate 1.15 Gbps, 236.44 Kpps input rate 1.15 Gbps, 236.83 Kpps; output rate 1.15 Gbps, 236.42 Kpps input rate 1.15 Gbps, 236.83 Kpps; output rate 1.15 Gbps, 236.92 Kpps input rate 1.15 Gbps, 236.25 Kpps; output rate 1.15 Gbps, 236.27 Kpps input rate 1.15 Gbps, 236.26 Kpps; output rate 1.15 Gbps, 236.26 Kpps input rate 1.15 Gbps, 236.26 Kpps; output rate 1.15 Gbps, 236.72 Kpps input rate 1.15 Gbps, 236.69 Kpps; output rate 1.15 Gbps, 236.72 Kpps input rate 1.15 Gbps, 236.69 Kpps; output rate 1.15 Gbps, 236.72 Kpps input rate 1.15 Gbps, 236.62 Kpps; output rate 1.15 Gbps, 236.72 Kpps input rate 1.15 Gbps, 236.26 Kpps; output rate 1.15 Gbps, 236.72 Kpps
input rate 968.63 Mbps, 49.26 Kpps; output rate 968.63 Mbps, 49.27 Kpps input rate 970.88 Mbps, 49.38 Kpps; output rate 970.89 Mbps, 49.38 Kpps input rate 968.61 Mbps, 49.32 Kpps; output rate 968.57 Mbps, 49.18 Kpps input rate 968.59 Mbps, 49.34 Kpps; output rate 970.81 Mbps, 49.29 Kpps input rate 968.59 Mbps, 49.18 Kpps; output rate 968.62 Mbps, 49.21 Kpps	input rate 1.15 Gbps, 236.70 Kpps; output rate 1.15 Gbps, 236.64 Kpps input rate 1.15 Gbps, 236.27 Kpps; output rate 1.15 Gbps, 236.23 Kpps input rate 1.15 Gbps, 236.67 Kpps; output rate 1.15 Gbps, 236.64 Kpps input rate 1.15 Gbps, 236.68 Kpps; output rate 1.15 Gbps, 236.03 Kpps input rate 1.15 Gbps, 236.58 Kpps; output rate 1.15 Gbps, 236.35 Kpps
input rate 970.82 Mbps, 49.29 Kpps; output rate 970.86 Mbps, 49.32 Kpps input rate 968.60 Mbps, 49.19 Kpps; output rate 968.64 Mbps, 49.26 Kpps input rate 970.84 Mbps, 49.30 Kpps; output rate 970.87 Mbps, 49.36 Kpps	input rate 1.15 Gbps, 236.11 Kpps; output rate 1.15 Gbps, 236.00 Kpps input rate 1.15 Gbps, 236.53 Kpps; output rate 1.15 Gbps, 236.43 Kpps



#### **Observations**

# Figure 41. 8 Node HPC Cluster comparison with HPGMG medium dataset test on 1 x NVIDIA A100-80G GPU vs Dual Socket CPU





The following observations were made from the test results obtained by running HPGMG medium dataset on the 8 x Cisco UCS C240 M7 node based HPC cluster as defined in this solution study:

- Depends on the workload and dataset size more GPU is required. HPGMG medium dataset consumed.
- The end-end FlexPod HPC cluster as highlighted in this solution scaled linearly whether the cluster test ran by CPU only or w/ GPU.
- Each node resources i.e., compute, storage and network consumed evenly throughout the cluster test.
- Compared to miniWeather and Minisweep test exercise above HPGMG medium dataset which is targeting application area of Cosmology, Astrophysics, Combustion showed 80% GPU utilization and 40% memory utilization.
- Due to the minimum memory required to execute the HPGMG medium dataset was higher than other two dataset we were not able to run the test on 1 GPU or 2 GPU in a single system.
- No CPU cycles were consumed when ran the test on NVIDIA A100-80G GPU.
- Time to complete the test with one GPU per node in an eight-node cluster is 3.5x faster than running the same test on eight-node cluster without GPU.

## Conclusion

The amalgamation of High-Performance Computing (HPC) and Artificial Intelligence (AI) represents a powerful synergy that unleashes unprecedented computational capabilities, enabling us to tackle complex and dataintensive challenges with greater speed, accuracy, and efficiency. The combination of CPUs and GPUs with high-speed data fabric with end-end 100GbE network is essential for achieving optimal performance, scalability, and responsiveness.

Here's the importance of each component because it allows for the best of HPC and Al worlds:

- **Diverse Workload Support:** CPUs are essential for handling diverse tasks, including system management, control flow, and sequential processes, making them crucial for both HPC and AI infrastructure.
- **Parallel Processing:** GPUs are vital for parallelizable workloads, such as deep learning and scientific simulations, where their massive parallel processing power accelerates complex calculations.
- **Task Offloading:** Combining CPUs and GPUs allows for intelligent task distribution, enabling CPUs to offload parallel workloads to GPUs for enhanced efficiency and speed.
- **Optimal Performance:** Together, CPUs and GPUs offer a balanced and high-performance computing environment, capable of handling a wide range of workloads seamlessly.
- **Energy Efficiency:** CPUs are generally more power-efficient for certain tasks and are important for overall system management. GPUs, on the other hand, excel in computational throughput. Combining the two can lead to better energy efficiency and performance.
- **Fast data pipeline:** Data intensive workloads of HPC and AI often involve large datasets. A 100GbE network provides an extensive data pipeline, ensuring efficient data exchange between CPUs, GPUs, storage rapidly and without bottlenecks, improving overall performance.
- Low Latency: Low-latency communication is crucial for HPC and AI workloads, as it reduces the time spent waiting for data transfers and results in faster overall processing.
- **Scalability:** High-speed networking supports the scaling of resources, enabling you to add more compute nodes, GPUs, or storage as needed for growing workloads.
- **Resource Utilization:** CPUs and GPUs are fully utilized as data moves quickly between them, minimizing idle times and maximizing the overall system efficiency.

In this solution study, we tested various application (use cases) targeted for weather simulation (miniWeather), Nuclear Engineering - Radiation Transport (Minisweep), and Cosmology, Astrophysics, Combustion (HPGMG).

We documented recommended tunable parameters to achieve balanced configuration amongst compute, network and storage components and proved near linear scalability of the solution as the size of the cluster grew from 1 to 8 node.

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## Appendix

This appendix contains the following:

- Appendix A Bill of Materials
- <u>Appendix B Cisco Nexus 9000 Switch Configuration</u>
- <u>Appendix C NetApp AFF A400 Storage Configuration</u>
- Appendix D Monitor GPU Utilization
- Appendix E References used in this guide
- <u>Appendix F Recommended for you</u>

## **Appendix A - Bill of Materials**

#### Cisco UCS C240 M7

Table 10 lists the bill of materials for the Cisco UCS C240 M7.

#### Cisco Nexus 93600CD-GX

Table 11 lists the bill of materials for the Cisco Nexus 93600CD-GX

#### Table 10. Bill of Material for Cisco UCS C240 M7

Part ID	Description	Qty
UCS-M7-MLB	UCS M7 RACK MLB	1
DC-MGT-SAAS	Cisco Intersight SaaS	1
DC-MGT-IS-SAAS-ES	Infrastructure Services SaaS/CVA - Essentials	8
SVS-DCM-SUPT-BAS	Basic Support for DCM	1
DC-MGT-UCSC-1S	UCS Central Per Server - 1 Server License	8
UCSC-C240-M7SX	UCS C240M7 Rack w/oCPU, mem, drv, 2Uw24SFF HDD/SSD backplane	8
UCSC-GPUAD-C240M7	GPU AIR DUCT FOR C240M7	8
UCS-M2-960G-D	960GB M.2 SATA Micron G2 SSD	16
UCS-M2-HWRAID-D	Cisco Boot optimized M.2 Raid controller	8
UCSX-TPM-002C-D	TPM 2.0, TCG, FIPS140-2, CC EAL4+ Certified, for servers	8
UCSC-RAIL-D	Ball Bearing Rail Kit for C220 & C240 M7 rack servers	8

Part ID	Description	Qty
CIMC-LATEST-D	IMC SW (Recommended) latest release for C-Series Servers.	8
UCSC-HSLP-C220M7	UCS C220 M7 Heatsink for & C240 GPU Heatsink	16
UCSC-BBLKD-M7	UCS C-Series M7 SFF drive blanking panel	176
UCS-DDR5-BLK	UCS DDR5 DIMM Blanks	128
UCSC-RISAB-24XM7	UCS C-Series M7 2U Air Blocker GPU only	8
CBL-FNVME-C240M7	C240M7 NVMe CABLE, MB P-4 to BP (NVMe 3-4)	8
UCSC-M2EXT-240-D	C240M7 2U M.2 Extender board	8
UCS-P100CBL-240-D	C240M7 NVIDIA P100 /A100 /A40 / A16 / A30 Cable	16
UCS-CPU-I6448H	Intel I6448H 2.4GHz/250W 32C/60MB DDR5 4800MT/s	16
UCS-MRX64G2RE1	64GB DDR5-4800 RDIMM 2Rx4 (16Gb)	128
UCSC-RIS1C-24XM7	UCS C-Series M7 2U Riser 1C PCle Gen5 (2x16)	8
UCSC-RIS2C-24XM7	UCS C-Series M7 2U Riser 2C PCle Gen5 (2x16) (CPU2)	8
UCSC-RIS3B-24XM7	UCS C-Series M7 2U Riser 3B support rear SAS & NVMe Drives	8
UCS-NVME4-1920-D	1.9TB 2.5in U.2 15mm P5520 Hg Perf Med End NVMe	32
UCSC-P-MCD100GF-D	Cisco-MLNX MCX623106AC-CDAT 2x100GbE QSFP56 PCIe NIC	8
UCSC-GPUA100-80-D	TESLA A100, PASSIVE, 300W, 80GB	8
NV-GRID-OPT-OUT-D	NVIDIA GRID SW OPT-OUT	8
UCSC-GPUA100-80-D	TESLA A100, PASSIVE, 300W, 80GB	8
NV-GRID-OPT-OUT-D	NVIDIA GRID SW OPT-OUT	8
UCSC-PSU1-2300W-D	Cisco UCS 2300W AC Power Supply for Rack Servers Titanium	16

Part ID	Description	Qty
CAB-C19-CBN	Cabinet Jumper Power Cord, 250 VAC 16A, C20-C19 Connectors	16
UCS-SID-INFR-UNK-D	Unknown	8
UCS-SID-WKL-UNK-D	Unknown	8
CON-OSP-UCSCPC34	SNTC-24X7X4OS UCS C240M7 Rack w/oCPU, mem, drv, 2Uw24S	8

#### Table 11. Bill of Material for Cisco Nexus 93600CD-GX

Part ID	Description	Qty
N9K-C93600CD-GX	Nexus 9300 with 28p 100G and 8p 400G	2
NXK-AF-PI	Dummy PID for Airflow Selection Port-side Intake	2
MODE-NXOS	Mode selection between ACI and NXOS	2
NXOS-9.3.10	Nexus 9500, 9300, 3000 Base NX- OS Software Rel 9.3.10	2
NXK-ACC-KIT-1RU	Nexus 3K/9K Fixed Accessory Kit, 1RU front and rear removal	2
NXA-FAN-35CFM-PI	Nexus Fan, 35CFM, port side intake airflow	12
NXA-PAC-1100W-PI2	Nexus AC 1100W PSU - Port Side Intake	4
CAB-C13-C14-AC	Power cord, C13 to C14 (recessed receptacle), 10A	4
C1-SUBS-OPTOUT	OPT OUT FOR "Default" DCN Subscription Selection	2
CON-SNC-N9KC936G	SNTC-NCD Nexus 9300 with 28p 100G and 8p 400G	2

## Appendix B - Cisco Nexus 9000 Switch Configuration

#### **Procedure 1.** Virtual Port-Channel (vPC) Configuration

A port channel bundles individual links into a channel group to create a single logical link that provides the aggregate bandwidth of up to eight physical links. If a member port within a port channel fails, traffic previously carried over the failed link switches to the remaining member ports within the port channel. Port channeling also load balances traffic across these physical interfaces. The port channel stays operational as long as at least one

physical interface within the port channel is operational. Using port channels, Cisco NX-OS provides wider bandwidth, redundancy, and load balancing across the channels.

In the Cisco Nexus Switch topology, a single vPC feature is enabled to provide HA, faster convergence in the event of a failure, and greater throughput. The Cisco Nexus vPC configurations with the vPC domains and corresponding vPC names and IDs for Oracle Database Servers are listed in <u>Table 12</u>.

Table 12. vPC Summary				
vPC Domain	vPC Name	vPC ID		
18	Peer-Link	1		
18	vPC Storage A	13		
18	vPC Storage B	14		

As listed in <u>Table 12</u>, a single vPC domain with Domain ID 1 is created across two Nexus switches to define vPC members to carry specific VLAN network traffic. In this topology, we defined a total number of 11 vPCs.

vPC ID 1 is defined as Peer link communication between the two Cisco Nexus switches. vPC IDs 13 and 14 are configured between both Cisco Nexus Switches and NetApp Storage Controller. vPC IDs 71-78 are configured between Mellanox ConnectX-6 Ehternet network interface card (NIC) ports on each Cisco UCS C240 M7 server connecting to Cisco Nexus Switches.





## Procedure 2. Create Virtual Port-Channel Domain

Step 1. Login as admin user into the Cisco Nexus A switch, run the following commands:

vpc domain 18

peer-keepalive destination 10.29.148.12 source 10.29.148.11

delay restore 150

peer-gateway auto-recovery ip arp synchronize role priority 10 Step 2. Login as admin user into the Cisco Nexus B switch, run the following commands: vpc domain 18 peer-keepalive destination 10.29.148.11 source 10.29.148.12 delay restore 150 peer-gateway auto-recovery ip arp synchronize role priority 20 interface Ethernet1/33 description Peer link connected to Leaf3-Spine1 switchport mode trunk switchport trunk allowed vlan 1,110,160,248 priority-flow-control mode on interface Ethernet1/34 description Peer link connected to Leaf3-Spine1 switchport mode trunk switchport trunk allowed vlan 1,110,160,248 priority-flow-control mode on interface Ethernet1/35 description Peer link connected to Leaf3-Spine2 switchport mode trunk switchport trunk allowed vlan 1,110,160,248 priority-flow-control mode on interface Ethernet1/36 description Peer link connected to Leaf3-Spine2 switchport mode trunk switchport trunk allowed vlan 1,110,160,248 **Step 1.** Repeat this procedure on Cisco Nexus B switch.

Procedure 3. Create Virtual Port-Channel between Cisco Nexus and NetApp Storage
Step 1. Login as admin user into the Cisco Nexus A switch, run the following commands
interface port-channel13
description PC-NetApp-A
switchport mode trunk
switchport trunk allowed vlan 110,160
spanning-tree port type edge trunk
mtu 9216
service-policy type qos input QOS_MARKING
vpc 13
no shutdown
interface port-channel14
description PC-NetApp-B
switchport mode trunk
switchport trunk allowed vlan 110,160
spanning-tree port type edge trunk
mtu 9216
service-policy type qos input QOS_MARKING
vpc 14
no shutdown
interface Ethernet1/27
description FlexPod-A400-CT1:e5a
switchport mode trunk
switchport trunk allowed vlan 110,160
mtu 9216
channel-group 13 mode active
no shutdown
interface Ethernet1/28
description FlexPod-A400-CT2:e5a
switchport mode trunk
switchport trunk allowed vlan 110,160
mtu 9216

channel-group 14 mode active

no shutdown

**Step 2.** Repeat this procedure on Cisco Nexus B switch for FlexPod-A400-CT1:e5b and FlexPod-A400-CT2:e5b

#### **Procedure 4.** Create Virtual Port-Channel between Cisco UCS C Series server and Cisco Nexus Switches

Step 1. Login as admin user into the Cisco Nexus A switch, run the following commands:

interface Ethernet1/3-10

switchport mode trunk

switchport trunk allowed vlan 110

priority-flow-control mode on

spanning-tree port type edge trunk

mtu 9216

service-policy type qos input QOS\_MARKING

no shutdown

**Step 2.** Repeat this procedure on the Cisco Nexus A switch for all C-Series rack servers with Mellanox ConnectX6-DX Ethernet NIC connected to Nexus 93600CD-GX

**Step 3.** Repeat this procedure on the Cisco Nexus B switch.

## Appendix C - NetApp AFF A400 Configuration

#### NetApp ONTAP 9.12.1

#### Procedure 1. Complete Configuration Worksheet

Before running the setup script, complete the Cluster setup worksheet in the NetApp ONTAP 9 Documentation Center. You must have access to the NetApp Support site to open the cluster setup worksheet.

#### **Tech tip**

It is beyond the scope of this document to explain the detailed information about the NetApp storage connectivity and infrastructure configuration. For installation and setup instruction for the NetApp AFF A400 System, go to: <a href="https://docs.netapp.com/us-en/ontap-systems/a400/index.html">https://docs.netapp.com/us-en/ontap-systems/a400/index.html</a>

For more information, visit FlexPod Design Guides: <u>https://www.cisco.com/c/en/us/solutions/design-zone/data-center-design-guides/flexpod-design-guides.html</u>

**Step 1.** For all the nodes data storage as part of the HPC cluster deployment, two large data aggregates (one aggregate on each storage node) were configured as shown below:
(aggr)	∟κ::> agǫ́	g snow					
Aggregate	Size	Available	Used%	State	#Vols	Nodes	RAID Status
A400_NVME_:	1 13.90TB	13.88TB	0%	online	9	A400-CLUSTER-01	raid_dp, normal
A400_NVME_2	13.90TB	13.88TB	0%	online	2	A400-CLUSTER-02	raid_dp, normal
	159.96B	7.75GB	95%	online	1	A400-CLUSTER-01	raid_dp, normal
4 entries v	159.9GB	7.75GB	95%	online	1	A400-CLUSTER-02	raid_dp, normal

**Step 2.** The screenshot below shows the Storage VMs (formally known as vserver) configured as "HPC-SVM" for this solution:

A400-CLUSTER::> vserver show							
	Tana	Out to an a	Admin	Operational	Root		
vserver	туре	Биртуре	State	State	volume	Aggregate	
A400-CLUSTER							
	admin						
A400-CLUSTER	R-01						
	node						
A400-CLUSTER	R-02						
	node						
HPC-SVM	data	default	running	running	HPC_SVM_ root	A400_NVME_ 2	
4 entries were displayed.							

**Step 3.** The SVM named "HPC-SVM" was configured to carry all NFS traffic for this HPC Data Analytics solution.



**Step 4.** Detailed configuration for HPC-SVM is shown below:

A400-CLUSTER::> vserver show -vserver HPC-SVM Vserver: HPC-SVM Vserver Type: data Vserver Subtype: default Vserver UUID: c6945eb3-576e-11ee-9e3e-d039ea33f86e Root Volume: HPC SVM root Aggregate: A400 NVME 2 NIS Domain: -Root Volume Security Style: unix LDAP Client: -Default Volume Language Code: C.UTF-8 Snapshot Policy: default Data Services: data-iscsi, data-nfs, data-nvme-tcp Comment: Quota Policy: default List of Aggregates Assigned: + Limit on Maximum Number of Volumes allowed: unlimited Vserver Admin State: running Vserver Operational State: running Vserver Operational State Stopped Reason: -Allowed Protocols: nfs, cifs, fcp, iscsi, ndmp, s3 Disallowed Protocols: nvme Is Vserver with Infinite Volume: false QoS Policy Group: -Caching Policy Name: -Config Lock: false IPspace Name: Default Foreground Process: -Logical Space Reporting: false Logical Space Enforcement: false Default Anti ransomware State of the Vserver's Volumes: disabled Enable Analytics on New Volumes: false Enable Activity Tracking on New Volumes: false

**Step 5.** The broadcast-domain was configured as "NFS-data" with MTU 9000 and assigned to default IPspace as shown below:

A400-CLUSTER::> network port broadcast-domain show								
Name	Domain Name	MTU	Port List	Status Details				
Cluster	Cluster	9000						
			A400-CLUSTER-02:e3a	complete				
			A400-CLUSTER-02:e3b	complete				
			A400-CLUSTER-01:e3a	complete				
			A400-CLUSTER-01:e3b	complete				
Default	Default	1500						
			A400-CLUSTER-02:e0M	complete				
			A400-CLUSTER-01:e0M	complete				
	NFS-data	9000						
			A400-CLUSTER-02:e5a	complete				
			A400-CLUSTER-02:e5a-110	complete				
			A400-CLUSTER-02:e5b	complete				
			A400-CLUSTER-02:e5b-110	complete				
			A400-CLUSTER-01:e5a	complete				
			A400-CLUSTER-01:e5a-110	complete				
			A400-CLUSTER-01:e5b	complete				
			A400-CLUSTER-01:e5b-110	complete				
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PRC	DTECTION V					Showing 1 - 11 of	11 Network Interfaces				<i>\</i>	1 ->	+	

**Step 7.** The export policy "default" was configured and added rules with clients subnets for UNIX systems to allow the NFSv4 protocol as shown below:

Step 8. Enable Cisco Discovery protocol.

A400-CLUSTER::> node run -node \* options cdpd.enable on

**Step 9.** Enable Link-Layer Discovery protocol on all ethernet ports:

A400-CLUSTER::> node run \* options lldp.enable on

### Appendix D - Monitor GPU Utilization

To monitor GPU utilization of our HPC cluster node while running different application; we created local Grafana dashboard for our solution test setup. This is for education purposes and recommended for lab/PoC only.

#### **Prerequisites**

- 1. Install and configure Grafana open-source server.
- 2. Verify Grafana server is running:

\$ sudo systemctl status grafana-server

Install Prometheus and configure Prometheus to run as service

#### 3. Verify that Prometheus is successfully installed using the below command:

\$ prometheus -version

\$ sudo systemctl start prometheus

sys

**Step 1.** Go to <u>http://<Grafana Server IP Address>:3000;</u> Log into Grafana using default username and password admin/password.

Welcome	e to Grafana
Email or username	
admin	
Password	
•••••	©
•••••	© Log in

- **Step 2.** Change the password when prompted.
- Step 3. Add Prometheus as data source.



Step 4. Add a new dashboard in Grafana. Go to home > Dashboard > new > import.

Ô		Q Search or jump to	≡ ctrl+k		+~   🗇	» 🖁
器 Dashboards	Dashboards Create and manage dashboar	ds to visualize your data				
Playlists Snapshots	Q Search for dashboards and	d folders			New	~
Library panels	S Filter by tag 🗸	Starred		t≡ Sort	New dashboa New folder	ard
	General				Import	

**Step 5.** Copy Grafana Dashboard ID "14574" for Nvidia GPU Metris: <u>https://grafana.com/grafana/dashboards/14574-nvidia-gpu-metrics/</u>

Step 6. Enter the Dashboard ID in Import via Grafana.com; click Load.

Ø		Q Search or jump to	🕮 ctrl+k
	port dashboard		
器 Dashboards	Import dashboard from file or	a <b>rd</b> Grafana.com	
Playlists Snapshots Library panels	D	L Upload dashboard JSON file rag and drop here or click to browse Accepted file types: .json, .txt	
	14574		Load
	Import via panel json		

Step 7. Edit /etc/prometheus/prometheus.yml file as shown in the example below:

\$ sudo vi /etc/prometheus/prometheus.yml

# my global config

global:

scrape\_interval: 15s # Set the scrape interval to every 15 seconds. Default is every 1 minute.

evaluation\_interval: 15s # Evaluate rules every 15 seconds. The default is every 1 minute.

# scrape\_timeout is set to the global default (10s).

# Alertmanager configuration

alerting:

alertmanagers:

- static\_configs:

- targets:
- # alertmanager:9093

# Load rules once and periodically evaluate them according to the global 'evaluation\_interval'.

rule\_files:

# - " first\_rules.yml"

# - "second\_rules.yml"

# A scrape configuration containing exactly one endpoint to scrape:

# Here it's Prometheus itself.

scrape\_configs:

# The job name is added as a label `job=<job\_name>` to any timeseries scraped from this config.

- job\_name: "prometheus"

# metrics\_path defaults to '/metrics'

# scheme defaults to 'http'.

static\_configs:

- targets: [" 10.29.148.171:9835" ]
- targets: ["10.29.148.172:9835"]
- targets: [" 10.29.148.173:9835" ]
- targets: [" 10.29.148.174:9835" ]
- targets: [" 10.29.148.175:9835" ]
- targets: [" 10.29.148.176:9835" ]
- targets: [" 10.29.148.177:9835" ]
- targets: [" 10.29.148.178:9835" ]

Step 8. Download node exporter from GitHub:

https://github.com/utkuozdemir/nvidia\_gpu\_exporter/releases

**Step 9.** On each client node install nvidia-gpu-exporter; for example:

\$ sudo dpkg -i nvidia-gpu-exporter\_1.2.0\_linux\_amd64.deb

**Step 10.** Log into Grafana webUI; go to dashboard created for Grafana. From the drop-down list next to GPU allows to switch between different GPU monitoring.

	› Nvidia GPU Metrics ☆ ペ	<b>⊪l∻</b> Add ~ 🛱 🛞	① Last 30 minutes - 오
GPU 01df8144-ddc2-303a-e7c8-ae12c571f85d ~			
Name © P-S © NVIDIA A100 80GB PCIe PO	GPU Utilizati   Power Draw %	Fan Speed % () Temperature ()	Memory Utilization % ③ 100% 75%
Driver Version         O         Vbios Version         O           535.104.05         92.00.A0.00.05	(0%) (15.1%)	(No data) (34 °C)	25%
Throttle Reasons ①	GPU Clock S         O         Memory Cloc         O           14.9%         100%         10%	Memory Alle © Memory Utili © 0.00488% 0%	GPU Utilization % ① 100% 75% 25% 0% 18:20 18:30 18:40
Memory Allocation ③ 5 M8 4 M8 3 M8 2 M8 1 M8 0 B 18:20 18:30 18:40	Temperature         O           100 °C	Power Draw () 50 W 40 W 30 W 20 W 10 W 0.W 18:20 18:30 18:40	Fan Speed %         O           100%         75%         No.data           55%         25%         0%           0%         18:20         18:30         18:40
Graphics Clock Speed ①	Video Clock Speed ①	SM Clock Speed ①	Memory Clock Speed

## Appendix E- References used in this guide

Anycast RP Technology White Paper:

https://www.cisco.com/c/en/us/td/docs/ios/solutions\_docs/ip\_multicast/White\_papers/anycast.html

Campus Network for High Availability Design Guide, Tuning for Optimized Convergence: <a href="https://www.cisco.com/c/en/us/td/docs/solutions/Enterprise/Campus/HA">https://www.cisco.com/c/en/us/td/docs/solutions/Enterprise/Campus/HA</a> campus DG/hacampusdg.html#wp1 107578

Campus Network for High Availability Design Guide: <u>https://www.cisco.com/c/en/us/td/docs/solutions/Enterprise/Campus/HA\_campus\_DG/hacampusdg.html</u>

## Appendix F - Recommended for you

Cisco Unified Computing System: <u>https://www.cisco.com/site/us/en/products/computing/servers-unified-</u> <u>computing-systems/index.html</u>

Cisco UCS 6536 Fabric Interconnects: <u>https://www.cisco.com/c/en/us/products/collateral/servers-unified-</u> computing/ucs6536-fabric-interconnect-ds.html

Cisco UCS X9508 Chassis: <u>https://www.cisco.com/c/en/us/products/collateral/servers-unified-</u> <u>computing/ucs-x-series-modular-system/datasheet-c78-2472574.html</u>

Cisco UCS X210c M7 Compute Node: <u>https://www.cisco.com/c/en/us/products/collateral/servers-unified-</u> computing/ucs-x-series-modular-system/ucs-x210c-m7-compute-node-ds.html

Cisco UCS X440p PCle Node: <u>https://www.cisco.com/c/en/us/products/collateral/servers-unified-</u> <u>computing/ucs-x-series-modular-system/ucs-x440p-pcle-node-ds.html</u>

Cisco UCS C240 M7 Rack Server: <u>https://www.cisco.com/c/en/us/products/collateral/servers-unified-computing/ucs-c-series-rack-servers/ucs-c240-m7-rack-server-ds.html</u>

Cisco UCS VIC 1500 Adapters: <u>https://www.cisco.com/c/en/us/products/collateral/interfaces-</u> modules/unified-computing-system-adapters/ucs-vic-15000-series-ds.html Cisco Intersight Infrastructure Service: <u>https://www.cisco.com/c/en/us/products/collateral/cloud-systems-</u> management/intersight/intersight-ds.html

Cisco UCS Manager: <u>https://www.cisco.com/c/en/us/products/servers-unified-computing/ucs-manager/index.html</u>

NVIDIA GPU Cloud: https://www.nvidia.com/en-us/gpu-cloud/

NVIDIA AI Enterprise: https://www.nvidia.com/en-us/data-center/products/ai-enterprise/

NVIDIA HPC SDK: <u>https://developer.nvidia.com/hpc-sdk</u>

Cisco Nexus 9300-GX Series Switch: <u>https://www.cisco.com/c/en/us/products/collateral/switches/nexus-9000-series-switches/nexus-9300-gx-series-switches-ds.html</u>

Cisco Nexus 9336C-FX2 Switch: <u>https://www.cisco.com/c/en/us/products/collateral/switches/nexus-9000-</u> series-switches/datasheet-c78-742282.html

NetApp Data ONTAP: <u>https://www.netapp.com/data-management/ontap-data-management-software/</u>

NetApp AFF A400: https://www.netapp.com/data-storage/aff-a-series/aff-a400/

SpecHPC 2021 Benchmark Suite: https://www.spec.org/hpc2021/

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