# Table of Contents

TR-4841: Hybrid Cloud AI Operating System with Data Caching ............................................ 1
  Use Case Overview and Problem Statement ................................................................. 1
  Solution Overview ......................................................................................................... 3
  Concepts and Components ........................................................................................... 6
  Hardware and Software Requirements ......................................................................... 9
  Solution Deployment and Validation Details .............................................................. 10
  Conclusion ..................................................................................................................... 22
  Acknowledgments ......................................................................................................... 22
  Where to Find Additional Information ........................................................................ 22
The explosive growth of data and the exponential growth of ML and AI have converged to create a zettabyte economy with unique development and implementation challenges.

Although it is a widely known that ML models are data-hungry and require high-performance data storage proximal to compute resources, in practice, it is not so straightforward to implement this model, especially with hybrid cloud and elastic compute instances. Massive quantities of data are usually stored in low-cost data lakes, where high-performance AI compute resources such as GPUs cannot efficiently access it. This problem is aggravated in a hybrid-cloud infrastructure where some workloads operate in the cloud and some are located on-premises or in a different HPC environment entirely.

In this document, we present a novel solution that allows IT professionals and data engineers to create a truly hybrid cloud AI platform with a topology-aware data hub that enables data scientists to instantly and automatically create a cache of their datasets in proximity to their compute resources, wherever they are located. As a result, not only can high-performance model training be accomplished, but additional benefits are created, including the collaboration of multiple AI practitioners, who have immediate access to dataset caches, versions, and lineages within a dataset version hub.

Next: Use Case Overview and Problem Statement

Use Case Overview and Problem Statement

Datasets and dataset versions are typically located in a data lake, such as NetApp StorageGrid object-based storage, which offers reduced cost and other operational advantages. Data scientists pull these datasets and engineer them in multiple steps to prepare them for training with a specific model, often creating multiple versions along the way. As the next step, the data scientist must pick optimized compute resources (GPUs, high-end CPU instances, an on-premises cluster, and so on) to run the model. The following figure depicts the lack of dataset proximity in an ML compute environment.
However, multiple training experiments must run in parallel in different compute environments, each of which require a download of the dataset from the data lake, which is an expensive and time-consuming process. Proximity of the dataset to the compute environment (especially for a hybrid cloud) is not guaranteed. In addition, other team members that run their own experiments with the same dataset must go through the same arduous process. Beyond the obvious slow data access, challenges include difficulties tracking dataset versions, dataset sharing, collaboration, and reproducibility.

Customer Requirements

Customer requirements can vary in order to achieve high-performance ML runs while efficiently using resources; for example, customers might require the following:

- Fast access to datasets from each compute instance executing the training model without incurring expensive downloads and data access complexities
- The use any compute instance (GPU or CPU) in the cloud or on-premises without concern for the location of the datasets
- Increased efficiency and productivity by running multiple training experiments in parallel with different compute resources on the same dataset without unnecessary delays and data latency
- Minimized compute instance costs
- Improved reproducibility with tools to keep records of the datasets, their lineage, versions, and other metadata details
- Enhanced sharing and collaboration so that any authorized member of the team can access the datasets and run experiments

To implement dataset caching with NetApp ONTAP data management software, customers must perform the following tasks:
• Configure and set the NFS storage that is closest to the compute resources.
• Determine which dataset and version to cache.
• Monitor the total memory committed to cached datasets and how much NFS storage is available for additional cache commits (for example, cache management).
• Age out of datasets in the cache if they have not been used in certain time. The default is one day; other configuration options are available.

Next: Solution Overview

Solution Overview

This section reviews a conventional data science pipeline and its drawbacks. It also presents the architecture of the proposed dataset caching solution.

Conventional Data Science Pipeline and Drawbacks

A typical sequence of ML model development and deployment involves iterative steps that include the following:

• Ingesting data
• Data preprocessing (creating multiple versions of the datasets)
• Running multiple experiments involving hyperparameter optimization, different models, and so on
• Deployment
• Monitoring

cnvrg.io has developed a comprehensive platform to automate all tasks from research to deployment. A small sample of dashboard screenshots pertaining to the pipeline is shown in the following figure.
It is very common to have multiple datasets in play from public repositories and private data. In addition, each dataset is likely to have multiple versions resulting from dataset cleanup or feature engineering. A dashboard that provides a dataset hub and a version hub is needed to make sure collaboration and consistency tools are available to the team, as can be seen in the following figure.
The next step in the pipeline is training, which requires multiple parallel instances of training models, each associated with a dataset and a certain compute instance. The binding of a dataset to a certain experiment with a certain compute instance is a challenge because it is possible that some experiments are performed by GPU instances from Amazon Web Services (AWS), while other experiments are performed by DGX-1 or DGX-2 instances on-premises. Other experiments might be executed in CPU servers in GCP, while the dataset location is not in reasonable proximity to the compute resources performing the training. A reasonable proximity would have full 10GbE or more low-latency connectivity from the dataset storage to the compute instance.

It is a common practice for data scientists to download the dataset to the compute instance performing the training and execute the experiment. However, there are several potential problems with this approach:

- When the data scientist downloads the dataset to a compute instance, there are no guarantees that the integrated compute storage is high performance (an example of a high-performance system would be the ONTAP AFF A800 NVMe solution).
- When the downloaded dataset resides in one compute node, storage can become a bottleneck when distributed models are executed over multiple nodes (unlike with NetApp ONTAP high-performance distributed storage).
- The next iteration of the training experiment might be performed in a different compute instance due to queue conflicts or priorities, again creating significant network distance from the dataset to the compute location.
- Other team members executing training experiments on the same compute cluster cannot share this dataset; each performs the (expensive) download of the dataset from an arbitrary location.
- If other datasets or versions of the same dataset are needed for the subsequent training jobs, the data scientists must again perform the (expensive) download of the dataset to the compute instance performing the training. NetApp and cnvrg.io have created a new dataset caching solution that eliminates these
hurdles. The solution creates accelerated execution of the ML pipeline by caching hot datasets on the ONTAP high-performance storage system. With ONTAP NFS, the datasets are cached once (and only once) in a data fabric powered by NetApp (such as AFF A800), which is collocated with the compute. As the NetApp ONTAP NFS high-speed storage can serve multiple ML compute nodes, the performance of the training models is optimized, bringing cost savings, productivity, and operational efficiency to the organization.

Solution Architecture

This solution from NetApp and cnvrg.io provides dataset caching, as shown in the following figure. Dataset caching allows data scientists to pick a desired dataset or dataset version and move it to the ONTAP NFS cache, which lies in proximity to the ML compute cluster. The data scientist can now run multiple experiments without incurring delays or downloads. In addition, all collaborating engineers can use the same dataset with the attached compute cluster (with the freedom to pick any node) without additional downloads from the data lake. The data scientists are offered a dashboard that tracks and monitors all datasets and versions and provides a view of which datasets were cached.

The cnvrg.io platform auto-detects aged datasets that have not been used for a certain time and evicts them from the cache, which maintains free NFS cache space for more frequently used datasets. It is important to note that dataset caching with ONTAP works in the cloud and on-premises, thus providing maximum flexibility.

Next: Concepts and Components

Concepts and Components

This section covers concepts and components associated with data caching in an ML workflow.
Machine Learning

ML is rapidly becoming essential to many businesses and organizations around the world. Therefore, IT and DevOps teams are now facing the challenge of standardizing ML workloads and provisioning cloud, on-premises, and hybrid compute resources that support the dynamic and intensive workflows that ML jobs and pipelines require.

Container-Based Machine Learning and Kubernetes

Containers are isolated user-space instances that run on top of a shared host operating system kernel. The adoption of containers is rapidly increasing. Containers offer many of the same application sandboxing benefits that virtual machines (VMs) offer. However, because the hypervisor and guest operating system layers that VMs rely on have been eliminated, containers are far more lightweight.

Containers also allow the efficient packaging of application dependencies, run times, and so on directly with an application. The most commonly used container packaging format is the Docker container. An application that has been containerized in the Docker container format can be executed on any machine that can run Docker containers. This is true even if the application’s dependencies are not present on the machine, because all dependencies are packaged in the container itself. For more information, visit the Docker website.

Kubernetes, the popular container orchestrator, allows data scientists to launch flexible, container-based jobs and pipelines. It also enables infrastructure teams to manage and monitor ML workloads in a single managed and cloud-native environment. For more information, visit the Kubernetes website.

cnvrg.io

cnvrg.io is an AI operating system that transforms the way enterprises manage, scale, and accelerate AI and data science development from research to production. The code-first platform is built by data scientists for data scientists and offers flexibility to run on-premises or in the cloud. With model management, MLOps, and continual ML solutions, cnvrg.io brings top-of-the-line technology to data science teams so they can spend less time on DevOps and focus on the real magic—algorithms. Since using cnvrg.io, teams across industries have gotten more models to production resulting in increased business value.

cnvrg.io Meta-Scheduler

cnvrg.io has a unique architecture that allows IT and engineers to attach different compute resources to the same control plane and have cnvrg.io manage ML jobs across all resources. This means that IT can attach multiple on-premises Kubernetes clusters, VM servers, and cloud accounts and run ML workloads on all resources, as shown in the following figure.
cnvrg.io Data Caching

cnvrg.io allows data scientists to define hot and cold dataset versions with its data-caching technology. By default, datasets are stored in a centralized object storage database. Then, data scientists can cache a specific data version on the selected compute resource to save time on download and thereby increase ML development and productivity. Datasets that are cached and are not in use for a few days are automatically cleared from the selected NFS. Caching and clearing the cache can be performed with a single click; no coding, IT, or DevOps work is required.

cnvrg.io Flows and ML Pipelines

cnvrg.io Flows is a tool for building production ML pipelines. Each component in a flow is a script/code running on a selected compute with a base docker image. This design enables data scientists and engineers to build a single pipeline that can run both on-premises and in the cloud. cnvrg.io makes sure data, parameters, and artifacts are moving between the different components. In addition, each flow is monitored and tracked for 100% reproducible data science.

cnvrg.io CORE

cnvrg.io CORE is a free platform for the data science community to help data scientists focus more on data science and less on DevOps. CORE’s flexible infrastructure gives data scientists the control to use any language, AI framework, or compute environment whether on-premises or in the cloud so they can do what they do best, build algorithms. cnvrg.io CORE can be easily installed with a single command on any Kubernetes cluster.

NetApp ONTAP AI

ONTAP AI is a data center reference architecture for ML and deep learning (DL) workloads that uses NetApp AFF storage systems and NVIDIA DGX systems with Tesla V100 GPUs. ONTAP AI is based on the industry-standard NFS file protocol over 100Gb Ethernet, providing customers with a high-performance ML/DL infrastructure that uses standard data center technologies to reduce implementation and administration overhead. Using standardized network and protocols enables ONTAP AI to integrate into hybrid cloud environments while maintaining operational consistency and simplicity. As a prevalidated infrastructure solution, ONTAP AI reduces deployment time and risk and reduces administration overhead significantly, allowing customers to realize faster time to value.

NVIDIA DeepOps

DeepOps is an open source project from NVIDIA that, by using Ansible, automates the deployment of GPU server clusters according to best practices. DeepOps is modular and can be used for various deployment tasks. For this document and the validation exercise that it describes, DeepOps is used to deploy a Kubernetes cluster that consists of GPU server worker nodes. For more information, visit the DeepOps website.

NetApp Trident

Trident is an open source storage orchestrator developed and maintained by NetApp that greatly simplifies the creation, management, and consumption of persistent storage for Kubernetes workloads. Trident itself a Kubernetes-native application—it runs directly within a Kubernetes cluster. With Trident, Kubernetes users (developers, data scientists, Kubernetes administrators, and so on) can create, manage, and interact with persistent storage volumes in the standard Kubernetes format that they are already familiar with. At the same time, they can take advantage of NetApp advanced data management capabilities and a data fabric that is powered by NetApp technology. Trident abstracts away the complexities of persistent storage and makes it simple to consume. For more information, visit the Trident website.
NetApp StorageGRID

NetApp StorageGRID is a software-defined object storage platform designed to meet these needs by providing simple, cloud-like storage that users can access using the S3 protocol. StorageGRID is a scale-out system designed to support multiple nodes across internet-connected sites, regardless of distance. With the intelligent policy engine of StorageGRID, users can choose erasure-coding objects across sites for geo-resiliency or object replication between remote sites to minimize WAN access latency. StorageGrid provides an excellent private-cloud primary object storage data lake in this solution.

NetApp Cloud Volumes ONTAP

NetApp Cloud Volumes ONTAP data management software delivers control, protection, and efficiency to user data with the flexibility of public cloud providers including AWS, Google Cloud Platform, and Microsoft Azure. Cloud Volumes ONTAP is cloud-native data management software built on the NetApp ONTAP storage software, providing users with a superior universal storage platform that addresses their cloud data needs. Having the same storage software in the cloud and on-premises provides users with the value of a data fabric without having to train IT staff in all-new methods to manage data.

For customers that are interested in hybrid cloud deployment models, Cloud Volumes ONTAP can provide the same capabilities and class-leading performance in most public clouds to provide a consistent and seamless user experience in any environment.

Next: Hardware and Software Requirements

Hardware and Software Requirements

This section covers the technology requirements for the ONTAP AI solution.

Hardware Requirements

Although hardware requirements depend on specific customer workloads, ONTAP AI can be deployed at any scale for data engineering, model training, and production inferencing from a single GPU up to rack-scale configurations for large-scale ML/DL operations. For more information about ONTAP AI, see the ONTAP AI website.

This solution was validated using a DGX-1 system for compute, a NetApp AFF A800 storage system, and Cisco Nexus 3232C for network connectivity. The AFF A800 used in this validation can support as many as 10 DGX-1 systems for most ML/DL workloads. The following figure shows the ONTAP AI topology used for model training in this validation.
To extend this solution to a public cloud, Cloud Volumes ONTAP can be deployed alongside cloud GPU compute resources and integrated into a hybrid cloud data fabric that enables customers to use whatever resources are appropriate for any given workload.

Software Requirements

The following table shows the specific software versions used in this solution validation.

<table>
<thead>
<tr>
<th>Component</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ubuntu</td>
<td>18.04.4 LTS</td>
</tr>
<tr>
<td>NVIDIA DGX OS</td>
<td>4.4.0</td>
</tr>
<tr>
<td>NVIDIA DeepOps</td>
<td>20.02.1</td>
</tr>
<tr>
<td>Kubernetes</td>
<td>1.15</td>
</tr>
<tr>
<td>Helm</td>
<td>3.1.0</td>
</tr>
<tr>
<td>cnvrg.io</td>
<td>3.0.0</td>
</tr>
<tr>
<td>NetApp ONTAP</td>
<td>9.6P4</td>
</tr>
</tbody>
</table>

For this solution validation, Kubernetes was deployed as a single-node cluster on the DGX-1 system. For large-scale deployments, independent Kubernetes master nodes should be deployed to provide high availability of management services as well as reserve valuable DGX resources for ML and DL workloads.

Next: Solution Deployment and Validation Details

Solution Deployment and Validation Details

The following sections discuss the details of solution deployment and validation.

Next: ONTAP AI Deployment
ONTAP AI Deployment

Deployment of ONTAP AI requires the installation and configuration of networking, compute, and storage hardware. Specific instructions for deployment of the ONTAP AI infrastructure are beyond the scope of this document. For detailed deployment information, see NVA-1121-DEPLOY: NetApp ONTAP AI, Powered by NVIDIA.

For this solution validation, a single volume was created and mounted to the DGX-1 system. That mount point was then mounted to the containers to make data accessible for training. For large-scale deployments, NetApp Trident automates the creation and mounting of volumes to eliminate administrative overhead and enable end-user management of resources.

Next: Kubernetes Deployment

Kubernetes Deployment

To deploy and configure your Kubernetes cluster with NVIDIA DeepOps, perform the following tasks from a deployment jump host:

1. Download NVIDIA DeepOps by following the instructions on the Getting Started page on the NVIDIA DeepOps GitHub site.
2. Deploy Kubernetes in your cluster by following the instructions on the Kubernetes Deployment Guide on the NVIDIA DeepOps GitHub site.

   For the DeepOps Kubernetes deployment to work, the same user must exist on all Kubernetes master and worker nodes.

   If the deployment fails, change the value of kubectl_localhost to false in deepops/config/group_vars/k8s-cluster.yml and repeat step 2. The Copy kubectl binary to ansible host task, which executes only when the value of kubectl_localhost is true, relies on the fetch Ansible module, which has known memory usage issues. These memory usage issues can sometimes cause the task to fail. If the task fails because of a memory issue, then the remainder of the deployment operation does not complete successfully.

   If the deployment completes successfully after you have changed the value of kubectl_localhost to false, then you must manually copy the kubectl binary from a Kubernetes master node to the deployment jump host. You can find the location of the kubectl binary on a specific master node by running the which kubectl command directly on that node.

Next: Cnvr.g.io Deployment

cnvr.g.io Deployment

Deploy cnvr.g CORE Using Helm

Helm is the easiest way to quickly deploy cnvr.g using any cluster, on-premises, Minikube, or on any cloud cluster (such as AKS, EKS, and GKE). This section describes how cnvr.g was installed on an on-premises (DGX-1) instance with Kubernetes installed.
Prerequisites

Before you can complete the installation, you must install and prepare the following dependencies on your local machine:

- Kubectl
- Helm 3.x
- Kubernetes cluster 1.15+

Deploy Using Helm

1. To download the most updated cnvrg helm charts, run the following command:

```
helm repo add cnvrg https://helm.cnvrg.io
helm repo update
```

2. Before you deploy cnvrg, you need the external IP address of the cluster and the name of the node on which you will deploy cnvrg. To deploy cnvrg on an on-premises Kubernetes cluster, run the following command:

```
helm install cnvrg cnvrg/cnvrg --timeout 1500s --wait \ --set
global.external_ip=<ip_of_cluster> \ --set global.node=<name_of_node>
```

3. Run the `helm install` command. All the services and systems automatically install on your cluster. The process can take up to 15 minutes.

4. The `helm install` command can take up to 10 minutes. When the deployment completes, go to the URL of your newly deployed cnvrg or add the new cluster as a resource inside your organization. The `helm` command informs you of the correct URL.

```
Thank you for installing cnvrg.io!
Your installation of cnvrg.io is now available, and can be reached via:
Talk to our team via email at
```

5. When the status of all the containers is running or complete, cnvrg has been successfully deployed. It should look similar to the following example output:
Computer Vision Model Training with ResNet50 and the Chest X-ray Dataset

cnvrg.io AI OS was deployed on a Kubernetes setup on a NetApp ONTAP AI architecture powered by the NVIDIA DGX system. For validation, we used the NIH Chest X-ray dataset consisting of de-identified images of chest x-rays. The images were in the PNG format. The data was provided by the NIH Clinical Center and is available through the NIH download site. We used a 250GB sample of the data with 627,615 images across 15 classes.

The dataset was uploaded to the cnvrg platform and was cached on an NFS export from the NetApp AFF A800 storage system.

Set up the Compute Resources

The cnvrg architecture and meta-scheduling capability allow engineers and IT professionals to attach different compute resources to a single platform. In our setup, we used the same cluster cnvrg that was deployed for running the deep-learning workloads. If you need to attach additional clusters, use the GUI, as shown in the following screenshot.
Load Data

To upload data to the cnvrg platform, you can use the GUI or the cnvrg CLI. For large datasets, NetApp recommends using the CLI because it is a strong, scalable, and reliable tool that can handle a large number of files.

To upload data, complete the following steps:

1. Download the cnvrg CLI.
2. Navigate to the x-ray directory.
3. Initialize the dataset in the platform with the `cnvrg data init` command.
4. Upload all contents of the directory to the central data lake with the `cnvrg data sync` command. After the data is uploaded to the central object store (StorageGRID, S3, or others), you can browse with the GUI. The following figure shows a loaded chest X-ray fibrosis image PNG file. In addition, cnvrg versions the data so that any model you build can be reproduced down to the data version.
Cach Data

To make training faster and avoid downloading 600k+ files for each model training and experiment, we used the data-caching feature after data was initially uploaded to the central data-lake object store.
After users click Cache, cnvrg downloads the data in its specific commit from the remote object store and caches it on the ONTAP NFS volume. After it completes, the data is available for instant training. In addition, if the data is not used for a few days (for model training or exploration, for example), cnvrg automatically clears the cache.

**Build an ML Pipeline with Cached Data**

cnvrg flows allows you to easily build production ML pipelines. Flows are flexible, can work for any kind of ML use case, and can be created through the GUI or code. Each component in a flow can run on a different compute resource with a different Docker image, which makes it possible to build hybrid cloud and optimized ML pipelines.
Building the Chest X-ray Flow: Setting Data

We added our dataset to a newly created flow. When adding the dataset, you can select the specific version (commit) and indicate whether you want the cached version. In this example, we selected the cached commit.
Building the Chest X-ray Flow: Setting Training Model: ResNet50

In the pipeline, you can add any kind of custom code you want. In cnvrg, there is also the AI library, a reusable ML components collection. In the AI library, there are algorithms, scripts, data sources, and other solutions that can be used in any ML or deep learning flow. In this example, we selected the prebuilt ResNet50 module. We used default parameters such as batch_size:128, epochs:10, and more. These parameters can be viewed in the AI Library docs. The following screenshot shows the new flow with the X-ray dataset connected to ResNet50.
Define the Compute Resource for ResNet50

Each algorithm or component in cnvrg flows can run on a different compute instance, with a different Docker image. In our setup, we wanted to run the training algorithm on the NVIDIA DGX systems with the NetApp ONTAP AI architecture. In The following figure, we selected `gpu-real`, which is a compute template and specification for our on-premises cluster. We also created a queue of templates and selected multiple templates. In this way, if the `gpu-real` resource cannot be allocated (if, for example, other data scientists are using it), then you can enable automatic cloud-bursting by adding a cloud provider template. The following screenshot shows the use of gpu-real as a compute node for ResNet50.
Tracking and Monitoring Results

After a flow is executed, cnvrg triggers the tracking and monitoring engine. Each run of a flow is automatically documented and updated in real time. Hyperparameters, metrics, resource usage (GPU utilization, and more), code version, artifacts, logs, and so on are automatically available in the Experiments section, as shown in the following two screenshots.
Conclusion

NetApp and cnvrg.io have partnered to offer customers a complete data management solution for ML and DL software development. ONTAP AI provides high-performance compute and storage for any scale of operation, and cnvrg.io software streamlines data science workflows and improves resource utilization.

Next: Acknowledgments

Acknowledgments

• Mike Oglesby, Technical Marketing Engineer, NetApp
• Santosh Rao, Senior Technical Director, NetApp

Next: Where to Find Additional Information

Where to Find Additional Information

To learn more about the information that is described in this document, see the following resources:

• Cnvrg.io (https://cnvrg.io):
  ◦ Cnvrg CORE (free ML platform)
    https://cnvrg.io/platform/core
  ◦ Cnvrg docs
    https://app.cnvrg.io/docs

• NVIDIA DGX-1 servers:
  ◦ NVIDIA DGX-1 servers
  ◦ NVIDIA Tesla V100 Tensor Core GPU
  ◦ NVIDIA GPU Cloud (NGC)

• NetApp AFF systems:
  ◦ AFF datasheet
  ◦ NetApp FlashAdvantage for AFF
- ONTAP 9.x documentation
  

- NetApp FlexGroup technical report
  

- NetApp persistent storage for containers:
  - NetApp Trident
    
    https://netapp.io/persistent-storage-provisioner-for-kubernetes/

- NetApp Interoperability Matrix:
  - NetApp Interoperability Matrix Tool
    
    http://support.netapp.com/matrix

- ONTAP AI networking:
  - Cisco Nexus 3232C Switches
    
  - Mellanox Spectrum 2000 series switches
    

- ML framework and tools:
  - DALI
    
    https://github.com/NVIDIA/DALI
    
    https://www.tensorflow.org/
    
    https://eng.uber.com/horovod/
  - Enabling GPUs in the Container Runtime Ecosystem
    
    https://devblogs.nvidia.com/gpu-containers-runtime/
  - Docker
    
    https://docs.docker.com
  - Kubernetes
    
    https://kubernetes.io/docs/home/
  - NVIDIA DeepOps
https://github.com/NVIDIA/deepops

- Kubeflow
  
  http://www.kubeflow.org/

- Jupyter Notebook Server
  
  http://www.jupyter.org/

- Dataset and benchmarks:
  
  - NIH chest X-ray dataset
    
    https://nihcc.app.box.com/v/ChestXray-NIHCC
