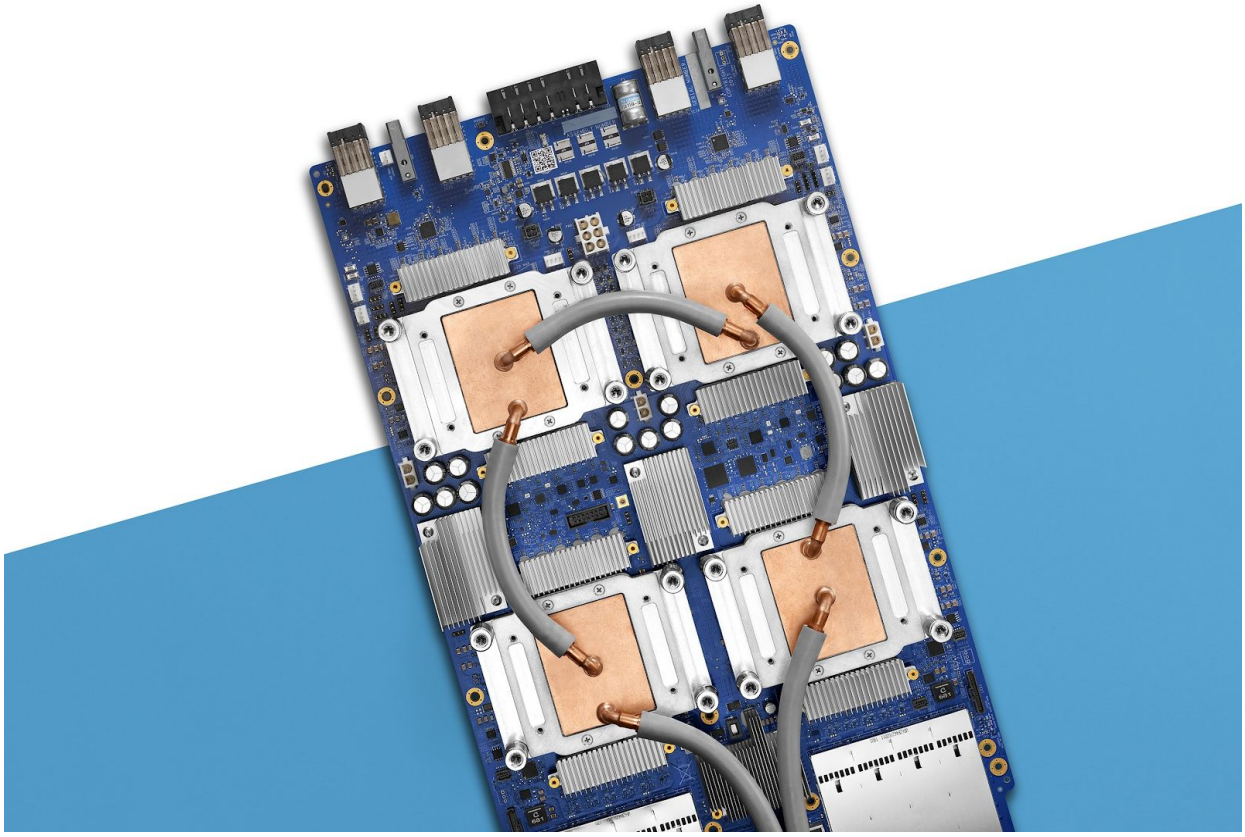
Google Cloud

High Performance Computing (HPC) Solutions in the Cloud

Cloud training, resources, and reference architectures for researchers and data scientists.



Google Cloud TPU v3

For more information visit **cloud.google.com/solutions/hpc/**

Contents

Introduction

The National Institutes of Health (NIH) established The Science and Technology Research Infrastructure for Discovery, Experimentation, and Sustainability (STRIDES) initiative to provide biomedical researchers with access to advanced, cost-effective, cloud-based computational infrastructure, tools, and services. Through STRIDES, researchers can take advantage of emerging data management methodologies, technological expertise, computational platforms, and tools to support cutting-edge experimentation and innovation. NIH has partnered with Google Cloud to support the STRIDES initiative through cloud services. In support of STRIDES, we've developed sets of playbooks to help enable researchers to build healthcare and life sciences solutions on Google Cloud Platform (GCP).

The goal of this playbook is to assist researchers in designing and implementing High Performance Computing workflows on GCP. More specifically, this playbook will focus on architecture and solutions examples for **building and storing singularity containers, hosting Jupyter notebooks in slurm clusters, setting up NFS file storage for Google Kubernetes Engine (GKE), and running TensorFlow inference workloads at scale**. Additionally, this playbook will outline training and digital resources to help upskill and enable researchers to build on Google Cloud, while highlighting the appropriate products and services to use when architecting on GCP.

Learning

Generally, cloud adopters fall under one of three categories:

Cloud Novice	Cloud Ready	Cloud Native
Little to no experience with the cloud	Familiar with the cloud, some experience	Lots of cloud experience, expert-level knowledge

Understanding this broad spectrum of experience levels, we've highlighted key training resources to help upskill researchers on Google Cloud. Additionally, Google offers on-site, instructor-led training to enable large groups of participants across your organization.

Cloud Novice

Video: Welcome to GCP

Video: Intro to GCP for Students

Video: GCP 101

Video: GCP Essentials

Documentation: GCP Conceptual Overview

Documentation: About GCP Services

Documentation: GCP Development & Admin Tools

Documentation: All GCP Products & Services

Virtual Course: GCP Fundamentals - Core Infrastructure

Virtual Lab: GCP Essentials

Cloud Ready

Documentation: All GCP Products & Services

Documentation: GCP for Data Center Professionals

Documentation: GCP for AWS Professionals

Documentation: GCP for Azure Professionals

Documentation: GCP for OpenStack Users

Video: Deploy an HPC Cluster

Video: Intro to HPC on GCP

Virtual Course: Intro to TensorFlow

Video: GPUs on GCP

Virtual Course: Essential Cloud Infrastructure - Foundation

Virtual Course: Essential Cloud Infrastructure - Core Services
Virtual Course: Elastic Cloud Infrastructure - Scaling and Automation

Virtual Course: Elastic Cloud Infrastructure - Containers and Services

Virtual Lab: Cloud Architecture

Virtual Lab: Cloud Engineering

VIrtual Lab: Cloud Development

Virtual Course: Architecting with Google Cloud Platform

Cloud Native

Documentation: All GCP Products & Services

Documentation: GCP Solutions

Documentation: Cloud Tensor Processing Units (TPUs)

Code Sample: HT Condor Deployment Manager Scripts

Codelab: Genomics Batch and High-Throughput Computing

Code Sample: Lustre Parallel File System Deployment Scripts

Video: Storage for HPC

Video: GPU Infrastructure for ML and HPC Workloads

Tutorial: Running R at Scale

Virtual Course: Machine Learning with TensorFlow

Virtual Lab: Intermediate ML: Tensorflow on GCP

Codelab: Image Processing & Astronomy

Virtual Course: Big Data and Machine Learning Fundamentals

Virtual Course: Leveraging Unstructured Data with Cloud Dataproc on Google Cloud Platform

Virtual Course: Serverless Data Analysis with Google BigQuery and Cloud Dataflow

Virtual Course: Serverless Machine Learning with Tensorflow on Google Cloud Platform

Virtual Course: Building Resilient Streaming Systems on GCP

Virtual Lab: Data Engineering

Virtual Lab: Data Science on GCP

Virtual Lab: Data Science on GCP - Machine Learning

Tutorial: Genomics GATK

Pipeline
Virtual Lab: Google Cloud Solutions II - Data and ML

Tutorial: TensorFlow Inference at Scale

High Performance Computing Solutions

Google offers powerful, flexible infrastructure capable of supporting scalable workloads. This allows researchers to work with data at a larger scale and faster than before, decreasing time from hypothesis to insight. GCP can enable and accelerate time to results for tasks from analyzing genomic sequence data to simulating complex climate models.

Compute, storage, and networking all operate at global scale at Google. Whether you need petabytes of storage or the latest processors, Google's infrastructure delivers. Build customized clusters with dozens of CPUs, powerful NVIDIA GPUs and Cloud Tensor Processing Units (TPUs), and high-throughput and low-latency object and file storage.

Cloud HPC solutions mean that every team has access to an effectively infinitely-scalable setup, tailored to their specific needs. This means less time waiting for workloads in queues, and more time for the work that really matters. For batch workloads, GCP offers the cloud-native Batch, providing dynamically-allocated compute clusters on Google Kubernetes Engine (GKE).

Google Cloud compute resources are billed at a per-second rate, meaning that you only pay for what you use. There are also a number of discounts available, such as automatically-applied Sustained Use Discounts, and up to 80% cost-savings with Preemptible VMs.

Tools such as BigQuery, AI Platform and Tensorflow enable researchers to apply analytics and artificial intelligence to data. Together with AutoML, users can establish mechanisms to auto-detect patterns, predict outcomes, and quickly analyze large amounts of data.

Additionally, both G Suite and GCP are FedRAMP compliant and HITRUST CSF certified; prescriptive security controls are implemented throughout Google Cloud for processing, storing, and transmitting sensitive data. Both G Suite and GCP also support HIPAA compliance across dozens of products in all regions, zones, network paths, and points of presence for Google Cloud.

Learn more about Google Cloud's high performance computing and innovative capabilities.

Reference Architectures

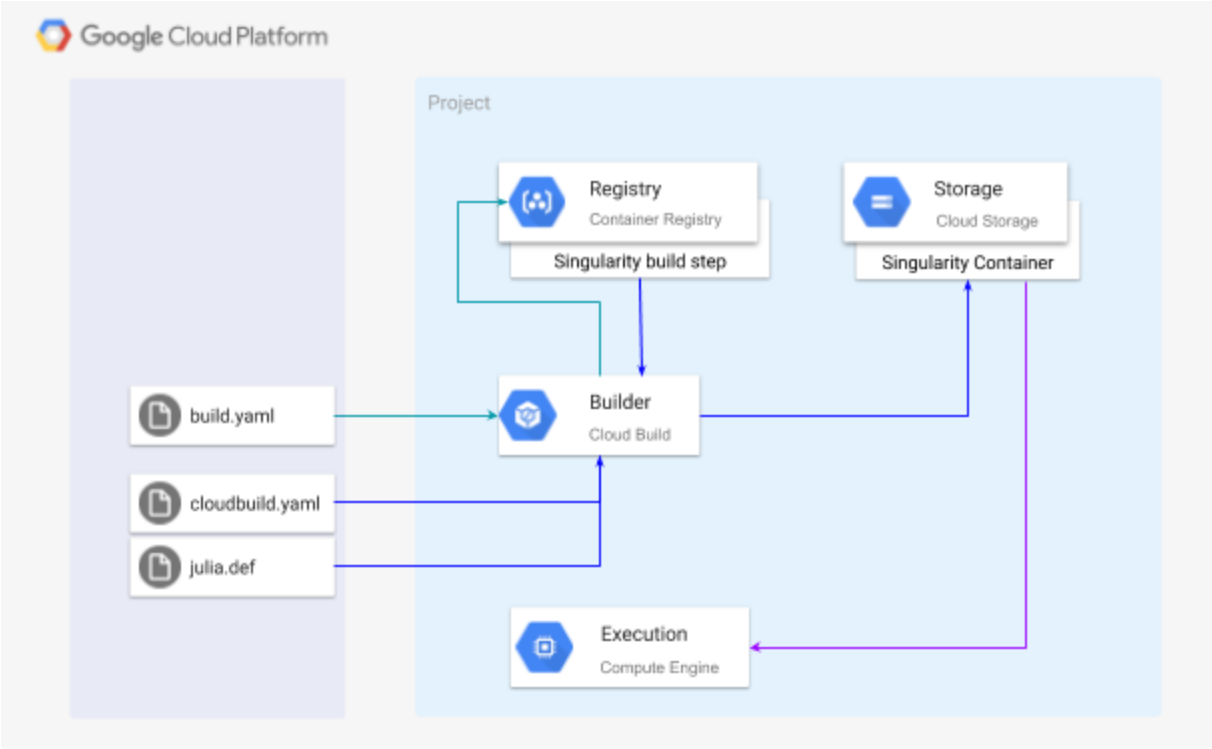
(link)

Google Cloud provides access to vastly scalable infrastructure backed by cutting-edge hardware to support your high performance workflows. Included here are a number of common HPC architectures and guidance on how to get them set up.

Singularity Containers with Cloud Build

(link)

Build, store, and deploy HPC-optimized Singularity containers on GCP with Cloud Build.



Solution Summary:

Use the cloud to configure and manage Singularity containers. Unlike Docker, the Singularity binary is specifically designed for HPC applications. Cloud Build provides a standard set of build steps which you can extend by creating your own specialized images. In this solution, we define a custom build step to build Singularity container images. We then use this to construct a Singularity container artifact and store it in Cloud Storage, before deploying to Compute Engine.

Suggested GCP Products and Services:

- Cloud VPC Network - Virtual Private Cloud provides global, scalable, and flexible networking for your GCP resources and services without compromising integrity on public-facing connections.
- Cloud Build - Executes your container builds on GCP infrastructure. Builds are run as a sequence of build steps, each within a Docker container. You can use provided build steps, or define your own custom ones.
- Container Registry - Private container image registry that runs on Google Cloud. Supports Docker Image Manifest V2 and OCI image formats.
- Cloud Storage - Unified object storage for storing raw data files and processed data. Supports regional, multi-regional, archive, and infrequently accessed data.
- Google Compute Engine (GCE) - VM instances for processing data.

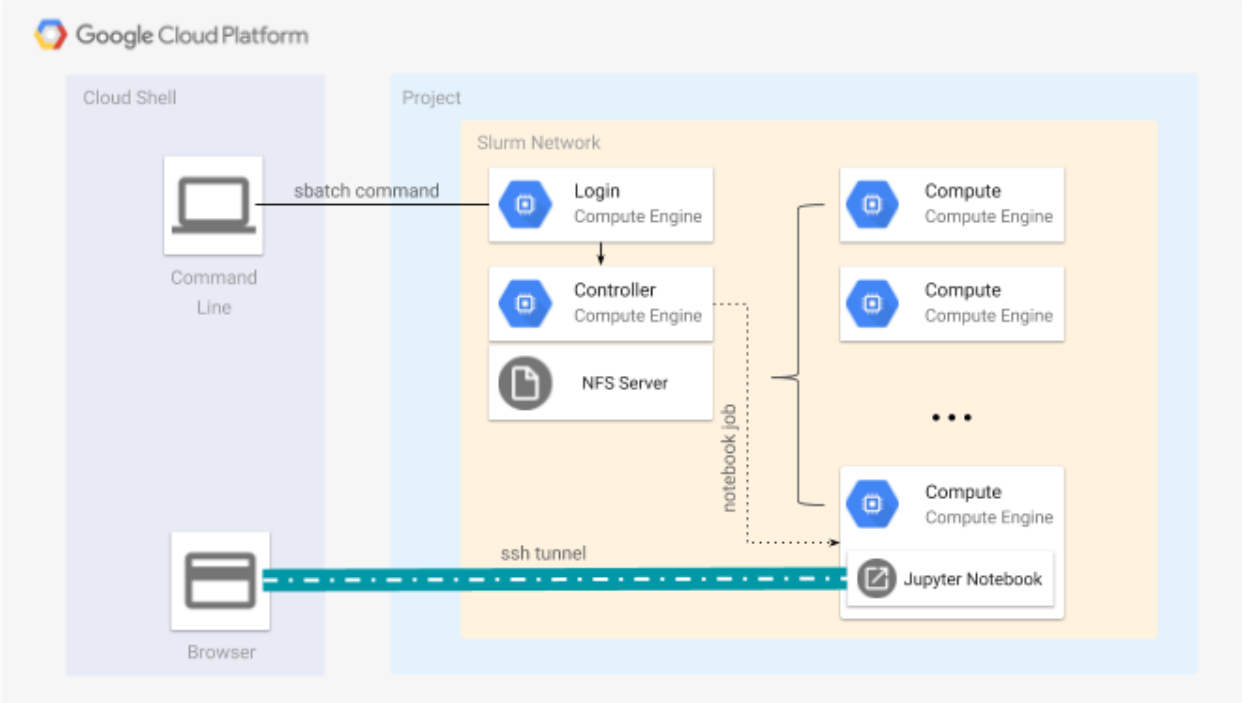
High-level Setup Steps:

1. Create a Google Cloud Project and use Cloud IAM to manage who has access to the resources within the GCP project.
2. Enable the Compute Engine, Cloud Build, and Container Registry APIs.
3. Define, and then build, a custom build step in `build.yaml` to create the Singularity builder.
4. Create a Cloud Storage bucket that will store the built container artifact. Note that you can use IAM to configure access policies to govern which workloads can access the containers you build.
5. Create a Singularity definition file (`julia.def`) to establish a blueprint for how the container will be constructed.
6. In `cloudbuild.yaml`, specify the steps required to build the container and store the result in a Cloud Storage bucket.
7. Use the custom Singularity build step created earlier together with `cloudbuild.yaml` and `julia.def` to build and store the container.
8. To deploy the container, first create a Compute Engine virtual machine with the `singularity` binary installed. Then, download the container from Cloud Storage and run it using `singularity`.

For code samples and a more detailed walkthrough, refer here.

Host Jupyter Notebooks in a Slurm Cluster

(link)
Run a Jupyter Notebook as a job managed by Slurm Workload Manager.



Solution Summary:

Slurm is a popular resource manager used in many high performance computing centers. Jupyter Notebooks are a favorite tool of machine learning and data science specialists. There are situations that call for specialized hardware, such as GPUs, or more memory or CPU cores than are available locally. In these situations, Slurm can allocate compute instances that have the required hardware resources to run the user's notebook for a bounded time period.

Suggested GCP Products and Services:

- Google Compute Engine (GCE) - VM instances for processing data.
- Deployment Manager - Infrastructure deployment service that automates the creation and management of Google Cloud resources.
- Cloud VPC Network - Virtual Private Cloud provides global, scalable, and flexible networking for your GCP resources and services without compromising integrity on public-facing connections.

High-level Setup Steps:

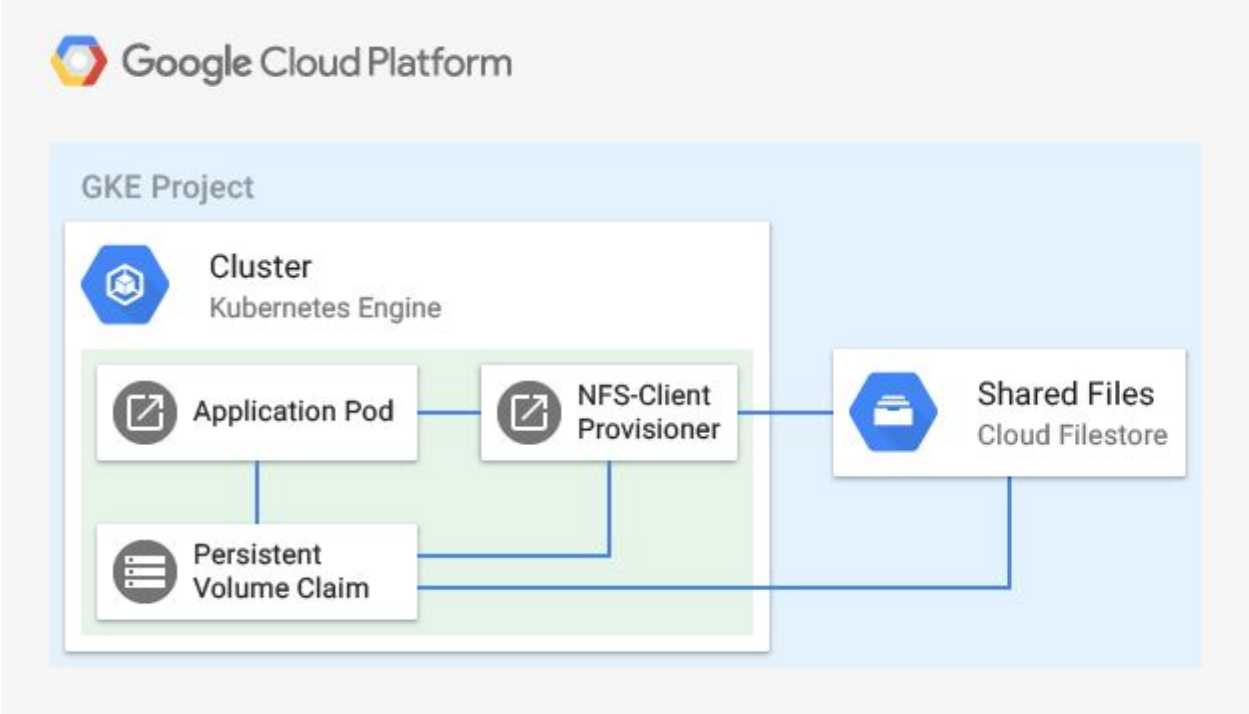
1. Create a Google Cloud Project and use Cloud IAM to manage who has access to the resources within the GCP project.
2. Enable the Compute Engine API.
3. Clone the Slurm on Google Cloud Platform GitHub repository, and customize the configuration for your environment.
4. Use Deployment Manager to deploy the Slurm Resource Manager to a Compute Engine cluster.
5. Setup an Anaconda environment module by installing the package on the controller, where each Slurm compute node can access it.
6. Run a Jupyter Notebook as a batch job on the Slurm cluster. This is done by submitting a `notebook.batch` file to Slurm via the `sbatch` command.
7. Establish an SSH tunnel to your Notebook via the Slurm login node. Use your browser to connect to your Notebook's interface through this tunnel. You now have a Jupyter Notebook up and running.

For code samples and a more detailed walkthrough, refer here.

GKE Dynamic Storage Provisioning from Cloud Filestore

(link)

Dynamically provision storage volumes in Google Kubernetes Engine (GKE) from Cloud Filestore using an NFS-Client Provisioner.



Solution Summary:

Dynamic provisioning allows storage volumes to be created on demand in an NFS volume managed by a Cloud Filestore instance. The NFS-Client Provisioner should be deployed to fulfil persistent volume storage claims from the application pods using Cloud Filestore's managed storage. Typical use cases include running databases, e.g., PostgreSQL, or a content management system like WordPress in a Kubernetes cluster.

Suggested GCP Products and Services:

- Google Kubernetes Engine - GKE provides a managed environment for deploying, managing, and scaling your containerized applications.
- Cloud Filestore - Managed file storage service for applications that require a filesystem interface and a shared file system for data, such as Network Attached Storage (NAS).

- Cloud VPC Network - Virtual Private Cloud provides global, scalable, and flexible networking for your GCP resources and services without compromising integrity on public-facing connections.

High-level Setup Steps:

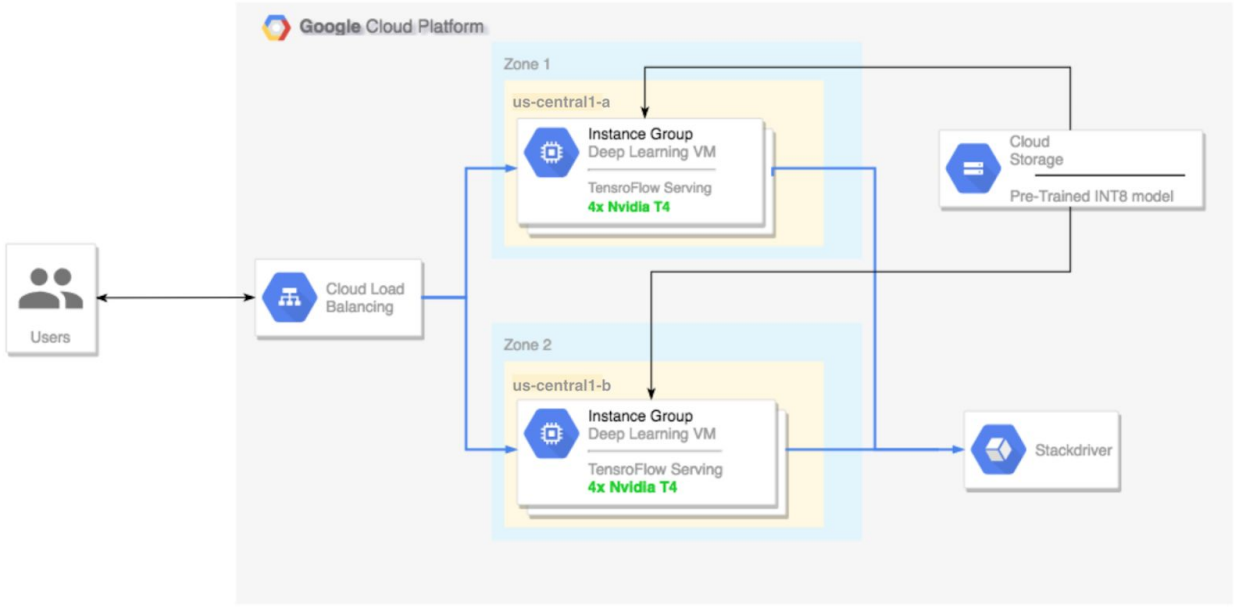
1. Create a Google Cloud Project and use Cloud IAM to manage who has access to the resources within the GCP project.
2. In the GCP project, create a VPC network to logically isolate your project resources.
3. Ensure the Cloud Filestore and GKE APIs are enabled.
4. Set up a Cloud Filestore storage volume.
5. Deploy a GKE cluster. This will host your application pods, and also the NFS-Client Provisioner.
6. Install the NFS-Client Provisioner using Helm and deploy it to the cluster.
7. You are up and running! Make a Persistent Volume Claim using any application that uses storage classes to do dynamic provisioning.
8. Optional: Verify Cloud Filestore volume directory creation by mounting the volume on a Compute Engine instance and inspecting the directory structure to see that the database files are present.

For code samples and a more detailed walkthrough, refer here.

TensorFlow Inference Workloads at Scale with TensorRT 5

(link)

Run deep learning inference on large-scale workloads with NVIDIA TensorRT 5 and NVIDIA T4 GPUs.



Solution Summary:

Set up a multi-zone cluster for running an inference workload on an autoscaling group that scales to meet changing GPU utilization demands. The Compute Engine VMs will be configured with Cloud Deep Learning VM images, and will serve the model using TensorFlow Serving.

Suggested GCP Products and Services:

- Google Compute Engine (GCE) - VM instances for processing data.
- Cloud Load Balancing - Distribute load-balanced compute resources in single or multiple regions, meet high availability requirements, put resources behind a single anycast IP and scale resources up or down with intelligent Autoscaling.
- Cloud Storage - Unified object storage for storing raw data files and processed data. Supports regional, multi-regional, archive, and infrequently accessed data.
- Stackdriver Monitoring - Collects metrics, events, and metadata from GCP, AWS, hosted uptime probes, and application instrumentation, as well as over 150 common application components, on-premise systems, and hybrid cloud systems.

- Cloud VPC Network - Virtual Private Cloud provides global, scalable, and flexible networking for your GCP resources and services without compromising integrity on public-facing connections.

High-level Setup Steps:

1. Create a Compute Engine VM configured with a TensorFlow Deep Learning image and in any zone that supports T4 GPUs.
2. Download and extract your TensorFlow SavedModel, before converting it to a TensorRT graph with TFTools.
3. Archive and upload the model to Cloud Storage, so that it can be served from the Compute Engine cluster later on.
4. Set up a multi-zone Compute Engine cluster:
    a. Prepare a startup script to install required services and libraries, such as NVIDIA drivers, GPU Utilization Agent, and TensorFlow Serving.
    b. Define an Instance Template.
    c. Create a Managed Instance Group.
    d. Configure Autoscaling using the GPU Utilization metric in Stackdriver.
5. Configure a Load Balancer in front of the Managed Instance Group. Ensure that firewall rules are set up to allow health checks by the Load Balancer, as well as HTTP traffic.
6. You can now POST model inputs to the TensorFlow Serving server using the Load Balancer's IP address to run GPU-backed inference and receive a prediction.

For code samples and a more detailed walkthrough, refer here.

Appendix

High Performance Computing Solutions Reference Architectures (link)

Technical Resources for HPC (link)

Reference Architecture for Creating a HIPAA-Aligned Project in GCP (link)

High Performance Computing - Google Cloud Blog (link)

Using Clusters for Large-Scale Technical Computing in the Cloud (link)

GCP Technical Tutorials (link)