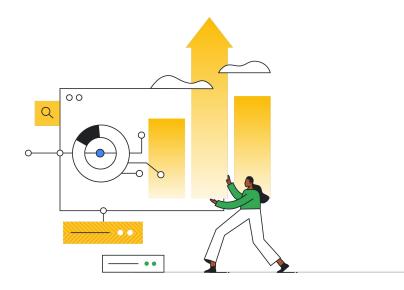
## Google Cloud

Build a flexible and powerful
High Performance Computing
foundation with
Google Cloud





**Volker Eyrich**Customer Engineer,
Google Cloud



**Joshua Fryer**Senior HPC Engineer,
Recursion

# Google Cloud helps meet your HPC needs with the fastest time to insight and simplicity



#### Fast and Affordable

- Latest HPC technologies
- Flexible VM shapes
- Batch VM types
- MPI scalability



# Easy and Compatible

- Simple and easy to use
- Turnkey HPC environments
- Compatible with leading apps and schedulers



#### Partner Preferred

- Broad ISV application support
- Broad network of Cloud HPC solution providers
- Broad ecosystem of HPC system integrators



#### Best of Google

- Industry expertise
- Leading ML and
- Data Analytics
- Hybrid & multi-cloud via Anthos/K8s
- Worldwide cloud network

# Deploy and manage HPC environments easily with Google Cloud's comprehensive platform

Google Cloud's HPC Platform



#### Users

Command Line Interface | Remote Workstations | Workbenches & Notebooks | HPC Platforms | API-Driven Workflows

#### **Deployment**

Scheduler, Deploy, Integrations, Monitoring, Marketplace

#### Development

Built-in Tools,
Communication
Libraries,
Infrastructure Mgmt

#### Infrastructure

Compute, Network, Storage

#### **Administrators**

VM-based | Google Cloud, Multi-Cloud, On-Premises Container-based | Google Cloud, Multi-Cloud, Private Cloud

# Google Cloud HPC Customers

#### **Enterprise HPC Customers**

























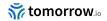












#### **Academic HPC Customers**





























# O1 HPC on Google Cloud

# Leverage Google Cloud's powerful HPC platform, tools, and partner solutions

#### Powerful Infrastructure

Compute Engine's VMs feature:

- Latest CPUs and GPUs
- High performance storage
- High throughput, low latency networking
- Live-migration, security built-in



#### **HPC Tools and Services**

Easily scale your workloads, run your containerized HPC workloads with GKE, and deploy auto-scaling HPC cluster environments with the Google Cloud HPC Toolkit

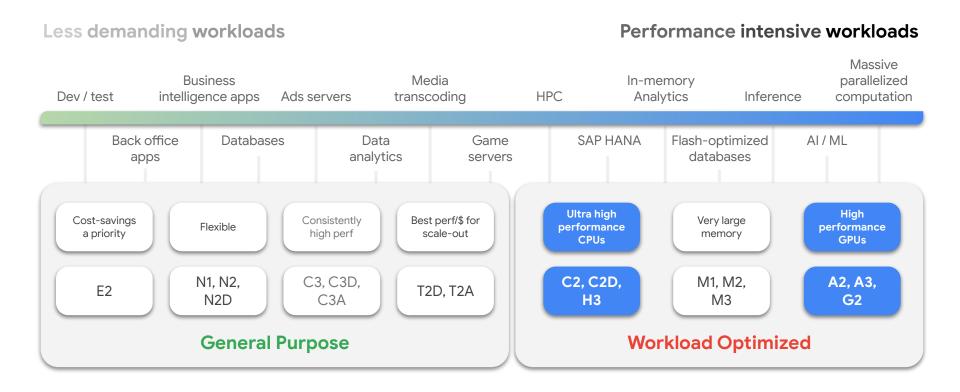


#### **Broad Partner Ecosystem**

Google partners with a wide variety of application developers, workload managers, storage providers, and system integrators

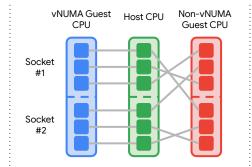


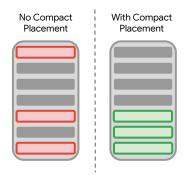
# VM Families Optimized for HPC Workloads

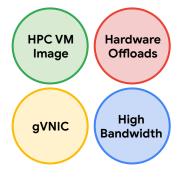


## What makes an HPC VM?









#### Purpose-built Infrastructure

Google Cloud's HPC VMs have the highest clock speeds and memory bandwidth of any Google VM type, as well as HPC features like disabling SMT. Choose from Intel or AMD CPUs.

#### Virtual NUMA (vNUMA)

vNUMA provides a direct mapping of Host CPU to Guest CPU and an accurate view of the NUMA layout of the guest on the host. Default on HPC VMs 2nd Gen and above.

#### Compact Placement

Compact placement policies put your VMs close together for low network latency between the VMs. Supports 100+ VMs per group. Supported by HPC VMs 2nd Gen and above.

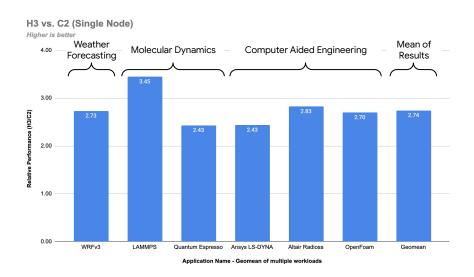
#### **Network Optimizations**

Google's HPC VMs perform optimally with our MPI best practice tunings in the HPC VM Image combined with our hardware offloads, high bandwidth VMs, and gVNIC drivers.

# Introducing H3 VMs for HPC

#### Now in Private Preview!

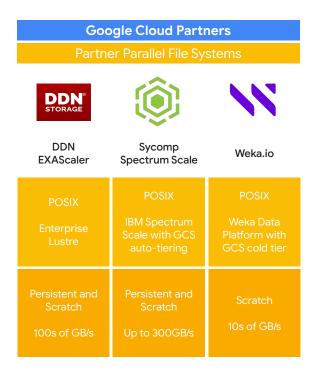
- Whole machine VM, full-core vCPUs, SMT off, 200 Gbps
- Intel Sapphire Rapids CPU, Intel IPU Hardware Offload
- Up to 3x better performance compared to prior gen
- 30-40% off the price of a similar C3 General Purpose VM





# HPC Storage on Google Cloud Object, Block, and File

| Google Cloud Services                      |  |   |   |
|--|--|---|---|
| Object                                     | File   | Parallel File                                     | File                                      |
| - •<br>- •                                 |  | -   |   |
| Cloud<br>Storage                           | Filestore  | Parallelstore                                     | NetApp<br>Volumes                         |
| JSON/S3<br>Unstructured<br>data, objects   | NFS<br>Enterprise and<br>High perf file<br>storage | POSIX, LibFS, KV  Next-gen DAOS-based HPC storage | NFS/SMB  Fully managed and featured ONTAP |
| Persistent<br>>> TB/s with<br>high latency | Persistent<br>26 GB/s with<br>low latency          | Scratch<br>>>TB/s with ultra<br>low latency       | Persistent<br>Up to 4.5GBs                |



### **Parallelstore**

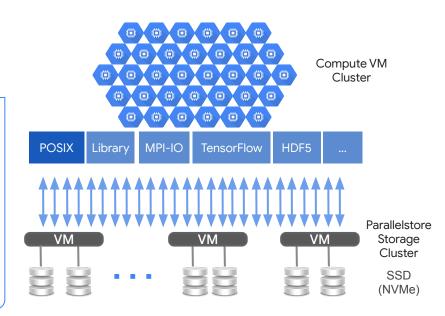
#### Next Gen HPC Storage System - Now in Private Preview!

Accelerate HPC and AI workloads that require extreme scale and/or low latency I/O operations



#### **Key Advantages**

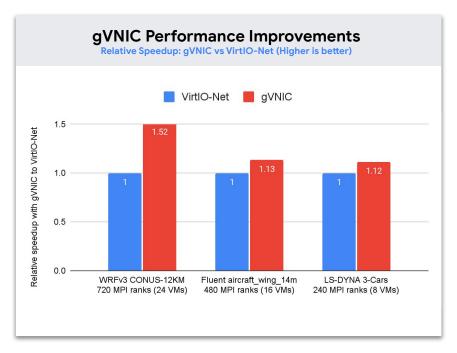
- Unique open-source DAOS storage architecture improves performance over existing POSIX storage options
- Standalone storage, or accelerate access to Cloud Storage
- Well-aligned to emerging patterns in Al workloads with distributed metadata, extreme IOPS, and K/V architecture
- Demonstrated >1GB/s per TiB, >1.5M create/s with open-source on GCP
  - Up to 6.3x of FSx Lustre read throughput of 200MB/s per TiB (Burst to 1,300)



# **HPC Networking on Google Cloud**

Scalable, high-bandwidth, low-latency VM networking

- Scalable VM Bandwidth
  - Up to 32 Gbps by default, 2 Gbps per vCPU
  - Up to 200 Gbps with 3rd Gen VM types
- Latency Tuning & Optimization
  - Predictable, low latency (<10 μs average)</li>
  - Google's HPC VM Image implements our MPI Best Practices and tunings
  - gVNIC Open Source Linux Kernel module built for GCE networking
  - Placement Policies allow compact colocation, reducing VM to VM latency
  - o **9K MTUs** (Jumbo Frames) increase packet size
- Up to 15,000 VMs per Virtual Private Cloud Network



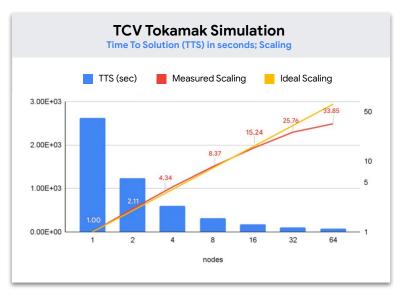
https://cloud.google.com/blog/topics/hpc/running-mpi-workloads-efficiently-on-google-cloud-using-gvnic

# Swiss Plasma Center on Google Cloud

"We can now deploy a flexible and powerful HPC infrastructure that is virtually identical to the one we maintain at EPFL in less than 15 minutes and dynamically offload on-prem workloads in times of high demand."

"Using Tokamak Configuration Variable (TCV) geometry, our results show excellent scalability: we managed to get a **33X** speedup for the TCV tokamak simulation, with a near-perfect scale up to 32 nodes."

- Swiss Plasma Center



https://cloud.google.com/blog/topics/hpc/swiss-plasma-center-uses-google-cloud-to-simulate-fusion

# How to run HPC on Google Cloud





Combine Google Cloud's HPC software, infrastructure, and partner solutions on your own to create your specific HPC environment. Configure, deploy, and maintain your HPC system yourself.



#### Cloud HPC Toolkit

Use Google's powerful, flexible Cloud HPC Toolkit to design and deploy a bespoke HPC environment leveraging Google's partner solutions, with Google's HPC best practices built in.



#### **HPC Platform Partner**

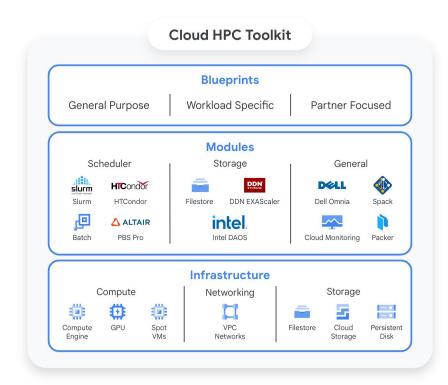
Leverage an HPC Platform provider that partners with Google Cloud to deliver out-of-the-box performance and reliability, combined with an easy-to-use web interface and application menu.

## **Cloud HPC Toolkit**

The Cloud HPC Toolkit is a modular, composable, terraform-based toolkit designed to make it easy to deploy repeatable, turnkey HPC environments that follow Google Cloud's HPC best practices.

#### **Key components:**

- Blueprints defines an HPC environment by importing and configuring individual modules which the toolkit assembles to build the specified environment
- Modules are pieces of code (imported from Github or locally) which deploy specific components of an HPC system (i.e. a project, network, VDI, Slurm controller)
- Infrastructure will host the HPC system that is built.
   The Cloud HPC Toolkit supports Google Cloud's latest and greatest HPC services and features out of the box



# Cloud HPC Toolkit Blueprint

```
blueprint_name: hpc-cluster-small

vars:
    project_id: ## Set GCP Project ID Here ##
    deployment_name: hpc-small
    region: us-central1
    zone: us-central1-c

deployment_groups:
    group: primary
    modules:
    id: network1
        source: modules/network/pre-existing-vpc
```



```
- id: homefs
 source: (...)/file-system/DDN-EXAScaler
 use: [network1]
- id: compute partition
 source: (...)/SchedMD-slurm-on-gcp-partition
 use: [ network1, homefs ]
 settings:
   partition name: compute
   max node count: 20
- id: slurm controller
 source: (...)/SchedMD-slurm-on-gcp-controller
 use: [ network1, homefs, compute partition ]
- id: slurm login
 source: (...)/SchedMD-slurm-on-gcp-login-node
 use: [ network1, homefs, slurm controller]
- id: hpc dash
 source: modules/monitoring/dashboard
```

# Journey to a working environment

From 40,269 lines to 62 **Deploy environment** Reads the deployment folder and provisions all of **HPC Environment** the infrastructure and Configuration software **Environments are** (40,269 lines) extended by editing a simple text file in YAML format (62 lines) Create deployment artifacts Based on the toolkit modules and the config file, generates the deployment folder containing provisioning code (3,626 lines)

## Cloud HPC Toolkit Blueprint for GROMACS

#### What was deployed?

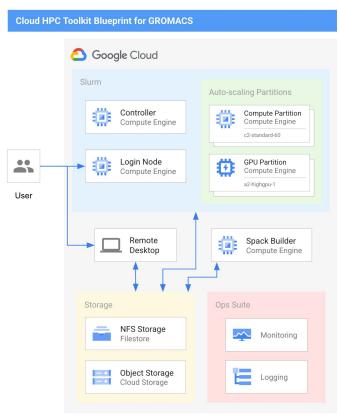
- APIs enabled. VPC network created
- Storage
  - GCS Buckets, Filestore (NFS)
- Spack
  - Builder installs Intel MPI, GCC, and GROMACS to Filestore
- Slurm Cluster
  - VMs: Login Node, Controller
  - Auto-scaling Partitions: CPU, GPU (A2 + NVIDIA A100)
  - Storage Mounted
- Remote Desktop VMs with GPU Acceleration
  - Chrome Remote Desktop, VMD
  - Storage Mounted
- HPC Monitoring Dashboard



**GROMACS Blueprint** 



Cloud HPC Toolkit GROMACS Demo Video



# Google & SchedMD

## Slurm on Google Cloud

Since 2017, Google has partnered with SchedMD to integrate the Slurm Workload Manager to harness the power of Google Cloud

#### Ways to use Slurm:

- Cloud Auto-Scaling: Automatic elastic scaling of instances, on demand, according to queue depth and job requirements. Spins resources down once idle timeout is reached.
- Hybrid Clusters: Extend your Slurm cluster to the cloud to dynamically offload jobs to Google Cloud using Cloud Auto-Scaling functionality. Accounting passed through from existing cluster.
- Enterprise support available directly from SchedMD
- Open Source from SchedMD:
   <a href="https://github.com/schedmd/slurm-qcp">https://github.com/schedmd/slurm-qcp</a>



# Slurm on Google Cloud v6

Improved feature functionality for Slurm on Google Cloud

- Support for the latest 3rd Gen and Arm VM families (C3, T2A)
- Full integration with the Google Cloud HPC Toolkit
- Enhanced error messages, actionable troubleshooting steps
- Improved job-level monitoring and reporting capabilities
- Reliability & update path enhancements
- Support for Shielded VMs for highly secure environments
- Expanded configuration options for auto-scaled VMs
- Enhancements to Slurm Hybrid capabilities
- Performance tunings for specific Slurm usage patterns
- TPU on Slurm support GA



## TPUs on Slurm v1

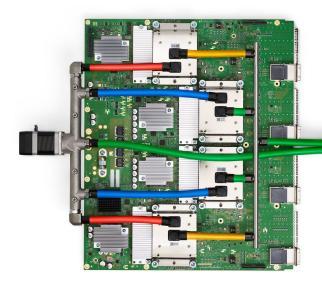
#### Support for Google Cloud TPUs in Slurm on GCP

#### Overview

- Define TPU-accelerated partitions like any other resource type
- Host TPU partitions alongside GPU partitions for Al workloads!
- Developed with input from major Al developers
  - o In use today by Al industry leaders, including Midjourney

#### **Features**

- Schedule and fair share across large TPU estates
- Deploy individual TPUs or TPU Pods
  - Supports TPU v2 and v3 today, v4+ coming soon!
- Supports PyTorch, JAX, and Tensorflow





# Integrating an On-Prem HPC cluster with Google Cloud:

**Power of Slurm** 

# Why Slurm for our HPC needs?



#### **Easy Integration**

Slurm WLM provides seamless integrations with Prometheus, Python, Open OnDemand and many more tools and applications

#### **SchedMD Support**

Various storage service offerings remove much of the burden of building and managing storage and infrastructure.



#### A Thriving Community

Widespread community knowledge with new Data Scientists and ML engineers already acquainted.

#### Freedom & Flexibility

**Enables streamlined pre-production testings,** hassle-free licensing, and lightweight operation.





RECURSION • BioHive 1





# **Expanding Horizons with Google Cloud**

# Google Cloud's HPC Platform



#### Scalability

GCP Offers real-time resource adjustment, seamless load distribution, and a global infrastructure for consistent performance worldwide. No more problematic nodes and hardware.

#### **Services and Tools**

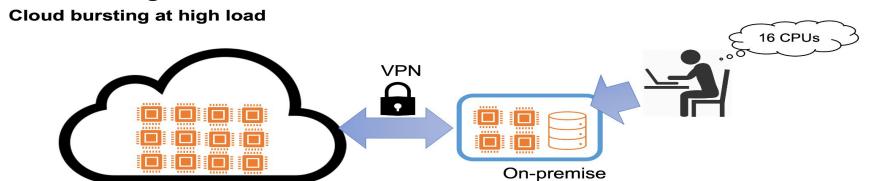
GCP provides powerful ML/AI tools, real-time big data analytics, and integrated cloud-based development environments for enhanced data processing and streamlined workflows. Supports tools like TF.

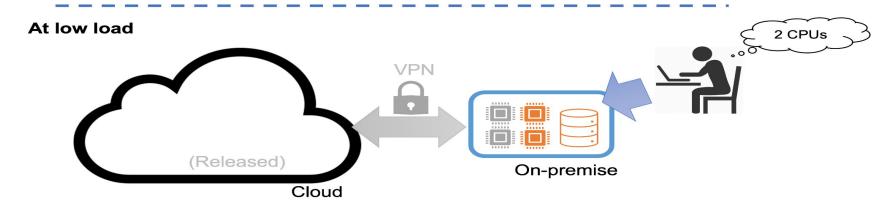
#### **Cost Optimization**

GCP offers a cost-effective model with pay-for-what-you-use flexibility, long-term usage discounts, and customizable resource options to match precise needs.

# Harnessing Best of Both Worlds

Cloud





# Thank you.