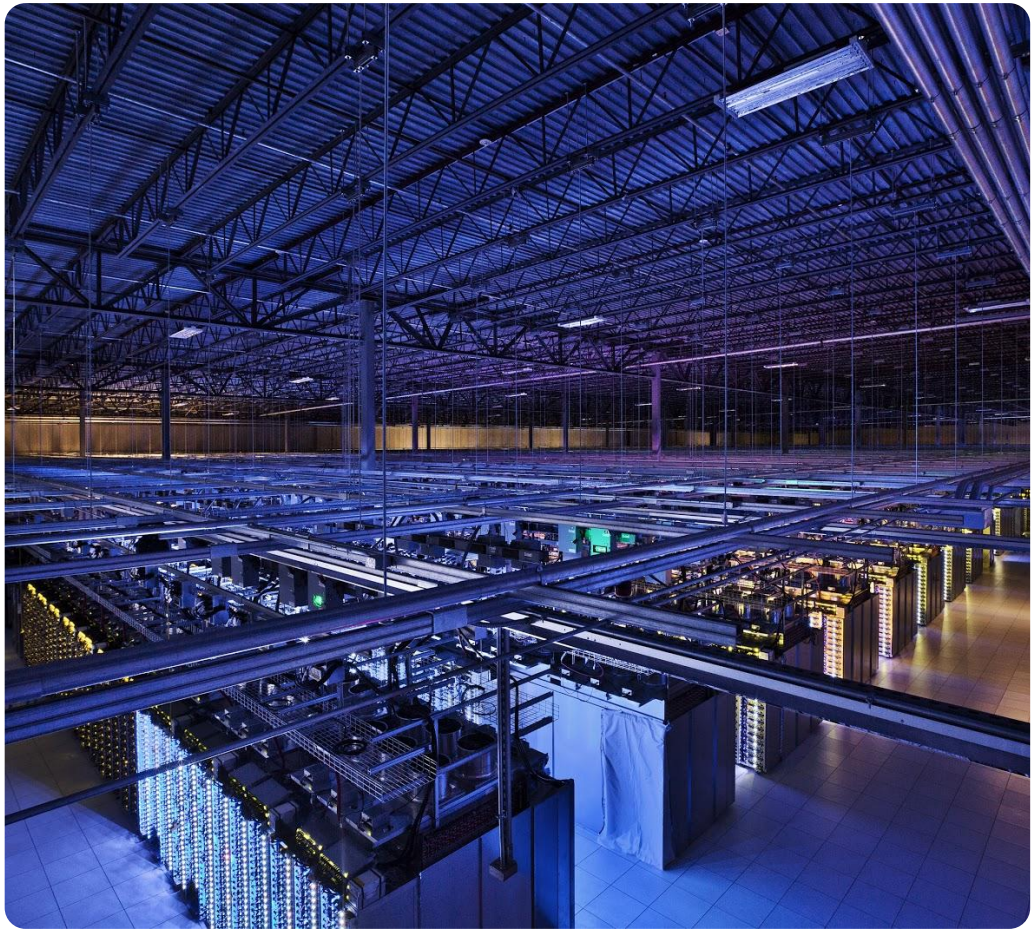
Scalable Research with Google Cloud HPC

Troy Sharpe
Customer Engineer
HPC
Google Cloud

Google Cloud



Agenda

01 What is Google Cloud HPC?

02 Google Cloud Infrastructure

03 HPC Software and Partnerships

04 Community and Getting Started

Cloud HPC Speeds Time to Insight

- Augment on-premises HPC with additional capacity
- Quickly access the latest technologies
- Accelerate new R&D with on-demand resources
- Enable worldwide collaboration

Google Cloud

Google's Unique HPC Capabilities

Hybrid, Standards-based HPC Environment
Cloud-capable, hybrid support for all major HPC schedulers and HPC platforms. Intel HPC standards-based, open source supporters.

High Performance Cloud Platform
Fastest VM creation in cloud. HPC-tuned VM types. Bulk API. 100Gbps, Placement Policies, and gVNIC for network-intensive workloads. High performance file, block, and object storage.

Unique Accelerator Types
Market-leading selection of NVIDIA GPUs, and Google's unique Cloud TPUs for purpose-built Machine Learning acceleration.

Scale and Resilience
Software-defined global network (lowest latency CSP), Cloud Storage with 11 nines of durability, VMs with seamless Live Migration.

Secure by Default
End-to-end encryption by default. Fully private environment built around Google's Zero Trust approach. Confidential Compute VMs.

HPC Simulation Platform

Google's HPC Simulation Platform

HPC Users

- Remote Workstations (VDI)
- Jupyter Notebooks
- Batch Schedulers
- API-Driven Workflows

Deployment

Integrations

ALTAIR, slurm, rescale, IBM Spectrum LSF, HTCondor, Parallel Works, CloudyCluster, NIMBIX

Purpose-Built

Life Sciences

Monitoring

Operations Suite

Marketplace

Cloud Marketplace

Development

Built-In Tools

HPC VM Images

HPC Toolkit

Message Passing Libraries

Intel MPI

Open MPI

Infrastructure Management

Terraform

Deployment Manager

Infrastructure

Compute

CPU, GPU, TPU, Spot

Network

Advanced Networking, Placement Policies, 9K MTU*

Storage

Filestore (NFS), Object Storage, Transfer Services, Storage Partners

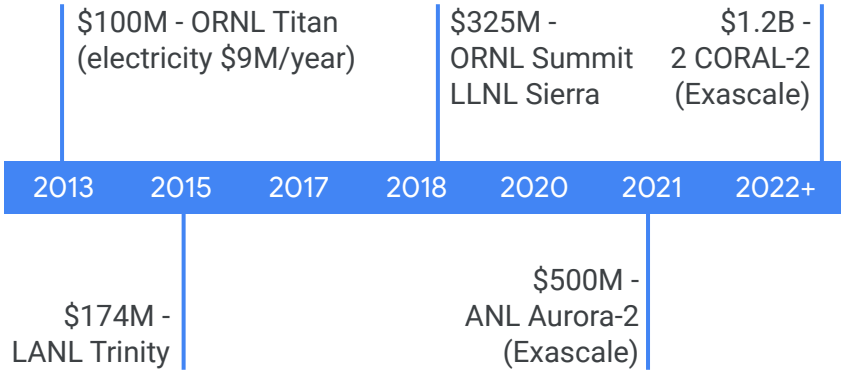
HPC Admins

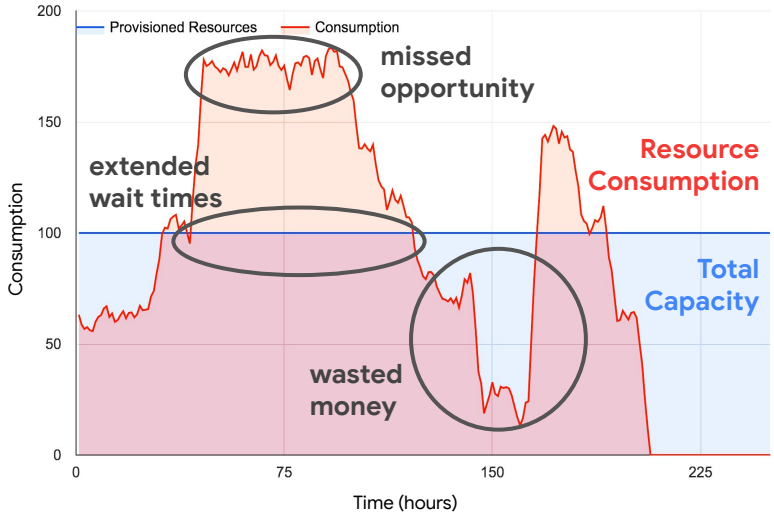
- VM-Based
  - Google Cloud
  - On-Premises
- Container-Based
  - Google Cloud
  - Multi-Cloud
  - Private Cloud

Google Cloud

Optimizing cost and resource utilization

CPU, GPU, Storage, Network, Servers, Building, Utilities, Cooling





Google Cloud

https://goo.gle/low-cost-hpc

Advancing climate science research.

Read the full case study

> We ran the job on 124,352 cores concurrently. We ran on 3,886 nodes. And we did that in 16.5 hours. The transition to GCP was enormously successful and greatly enhanced this research. It demonstrated that we could process these massive data sets in just a fraction of the time.
>
> **Paul Sagona**, Executive Director, Research Computing,
> University of South Carolina

The Molecular Microbial Biology Lab at the University of South Carolina cut its data processing time, and gained the tools and methods it needed to enhance its scientific research.

Challenge: Improve high-performance computing and data processing for scientific research.

Solution: The team mimicked its existing high-performance computing cluster on Google Cloud Platform, with flexible storage options and dynamically installed software that would scale with the data.

Results: Using Google Cloud, the research computing team helped the lab cut its data processing time from three months to 16 hours – allowing it to catch up on a year's backlog of data and show progress to help in winning research grants.

Google Cloud

UNIVERSITY OF SOUTH CAROLINA

Urgent HPC

Most researchers do not have access to the HPC resources needed to study complex systems

Traffic Management is a major hurdle to efficient emergency evacuations

Models of evacuation traffic patterns during hurricanes are valuable for evacuation planning

Reducing traffic congestion saves lives, time, money, and the environment

Google Cloud

Record-Breaking: 2.1M vCPUs

Clemson broke the world record for running an HPC workload using the most compute cores on any commercial cloud.

2.138M vCPU | 133, 573 instances | 210+ TB data processed

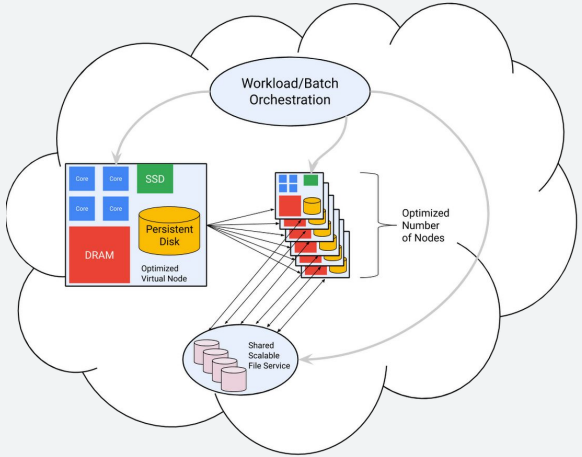
Average cost of **$0.008 USD per vCPU hour**

Published **“On-Demand Disaster Management using High Performance Computing in the Commercial Cloud,"** in The Journal of Supercomputing

A corpus of [traffic data for public use] is available via the Public Dataset Program

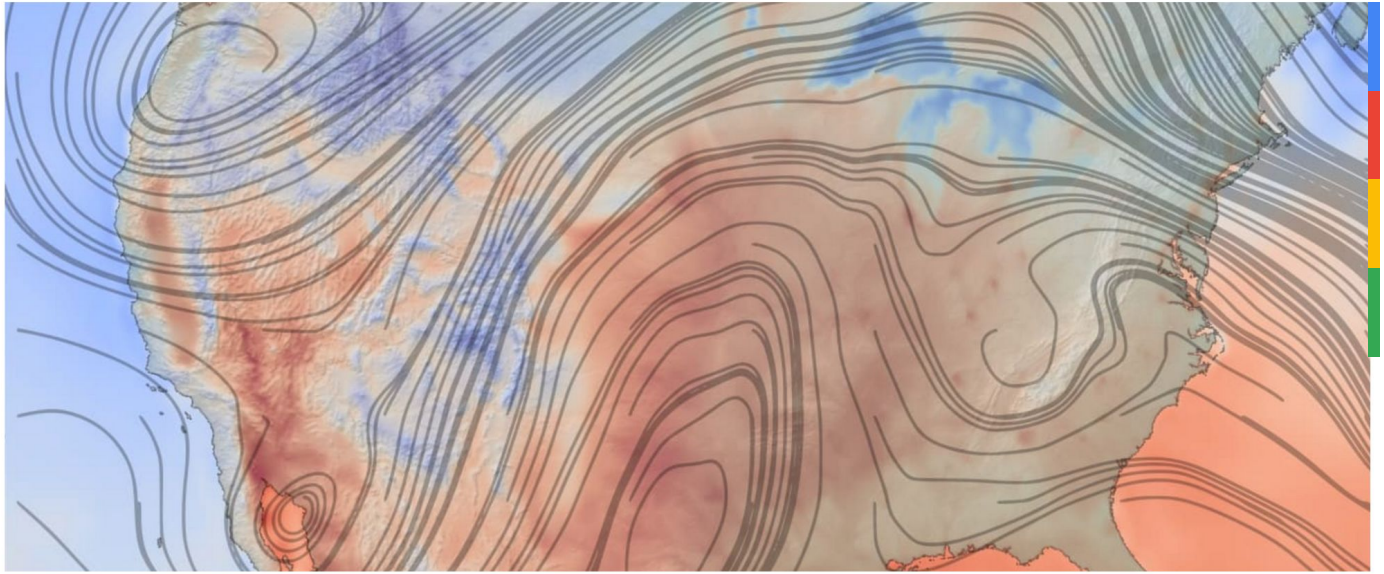
[Google Cloud Blog Post]

[10 Minute Lightning Talk - CloudHub]



Google Cloud

Clouds in the cloud: Weather forecasting in Google Cloud



Wyatt Gorman
HPC Solutions Manager, Google Cloud

Joe Schoonover
Founder & Director of Operations, Fluid Numerics

March 28, 2022

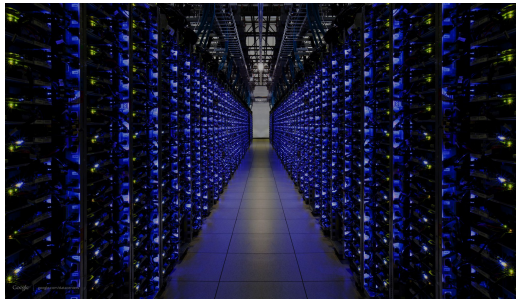
Weather forecasting and climate modeling are two of the world's most computationally complex and demanding tasks. Further, they're extremely time-sensitive and in high demand — everyone from weekend travelers to large-scale industrial farming operators wants up-to-date weather predictions. To provide timely and meaningful predictions, weather forecasters usually rely on high performance computing (HPC) clusters hosted in an on-premises data center. These on-prem HPC systems require significant capital investment and have high long-term operational costs. They

[Blog]

[CodeLab]

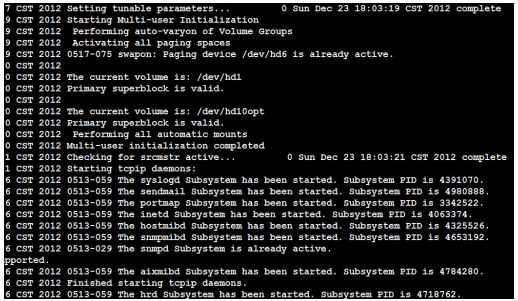
[Video Walkthrough]

Google



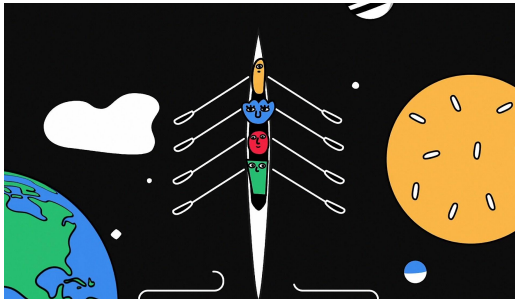
HPC Infrastructure

HPC is entering a new era defined by new accelerator technologies, rapidly enabling significant new advances.



HPC Software and Partnerships

Google's approach is towards open-source licensing, and partnering with popular vendors.

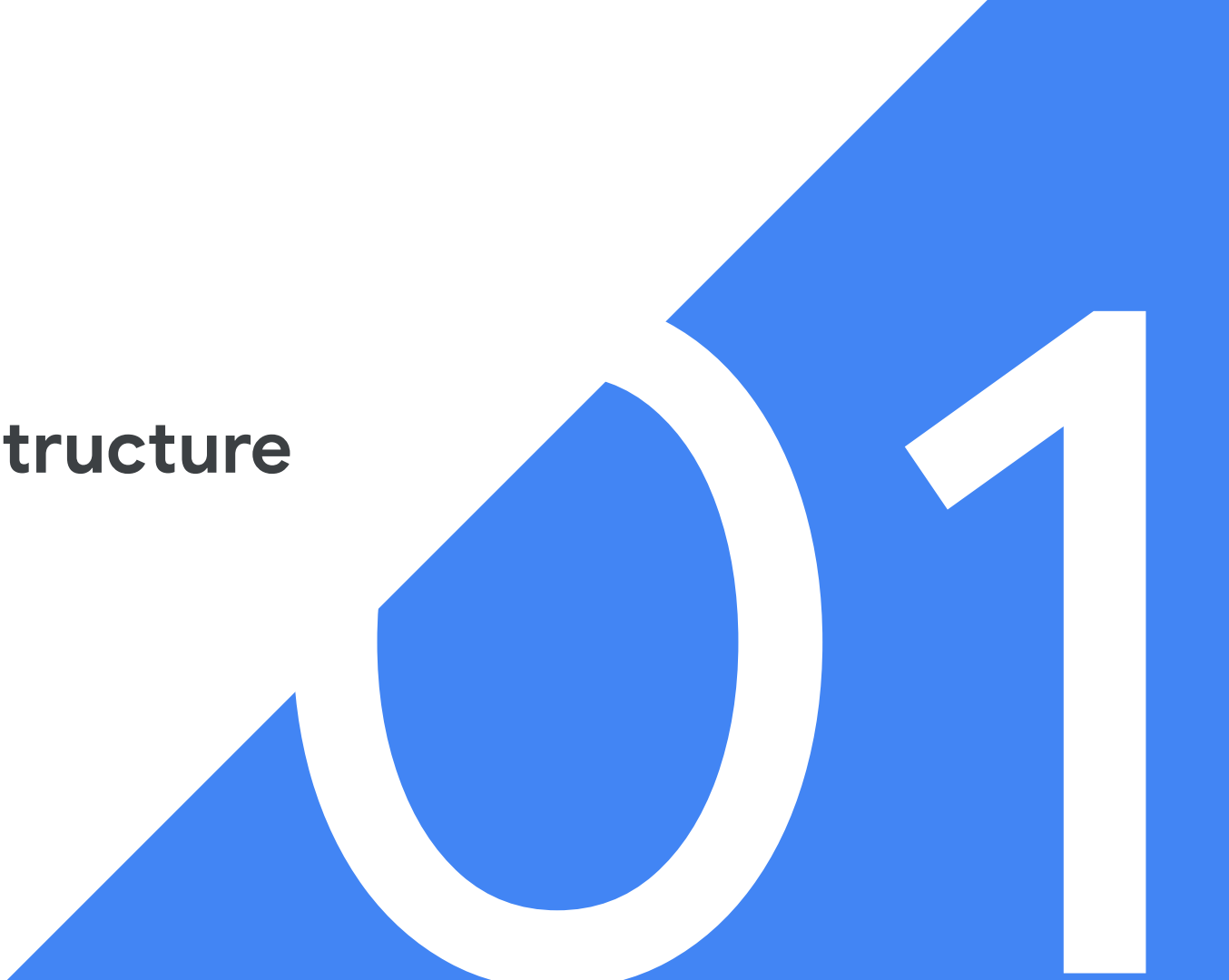


Community and Getting Started

Building new communities and engaging existing ones to partner together to democratize HPC.

Google Cloud

HPC Infrastructure

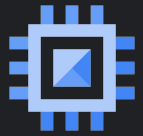


Google Cloud

Google Cloud Infrastructure

Our infrastructure in numbers

34 cloud regions (+9 announced regions) url
103 zones url
146 edge locations url
100+ CDN locations url
100+ Dedicated Interconnect locations url
19 subsea cable investments url
In **2022** we've launched **5** new region(s).



Compute

Google Cloud

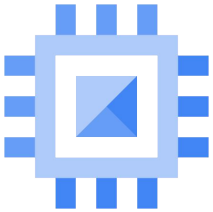
HPC Compute Building Blocks

HPC optimized, customizable, scalable, reliable instances

Purpose	General Purpose			Workload-Optimized		
Capability	Flexibility, GPUs	Balanced Performance	High Memory BW	Fastest Clock Speeds	Large, Fast Clocks	Large, A100 GPUs
Hardware Support (Up To)	• 48 cores (96 vCPU) • Intel Skylake thru Broadwell • 624GB RAM • 32Gbps • 9TB Local SSD • NVIDIA K80, T4, P4, P100, V100 • 4 or 8 GPUs • Supports TPUs	• 64 cores (128 vCPU) • Intel Cascade Lake or Ice Lake • 2.6GHz Base, 3.4GHz All-Core • 864GB RAM • 100Gbps • 9TB Local SSD	• 112 cores (224 vCPU) • AMD EPYC 2nd or 3rd Gen • 2.7GHz All-Core • 896GB RAM • 100Gbps • 9TB Local SSD	• 30 cores (60 vCPU) • Intel Cascade Lake • 3.8 GHz All-Core • 240GB RAM • 100Gbps • 3TB Local SSD • Compact Placement • vNUMA	• 56 cores (112 vCPU) • AMD EPYC 3rd Gen • 3.3GHz All-Core • 896GB RAM • 100Gbps • 3TB Local SSD • Compact Placement • vNUMA	• 48 cores (96 vCPU) • Intel Cascade Lake • 3.8 GHz All-Core • 1,360GB RAM • 100Gbps • 3TB Local SSD • Compact Placement • NVIDIA A100 (40GB) GPUs • 16 GPUs • NVSwitch @ 600GB/s • vNUMA
VM Series	**General Purpose (N1)**	**General Purpose (N2)**	**General Purpose (N2D)**	**Compute-Optimized (C2)**	**Compute-Optimized (C2D)**	**Accelerator-Optimized (A2)**

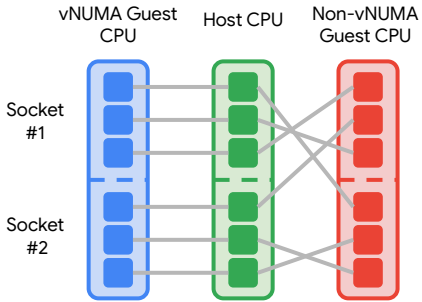
Google Cloud

What makes an HPC VM?



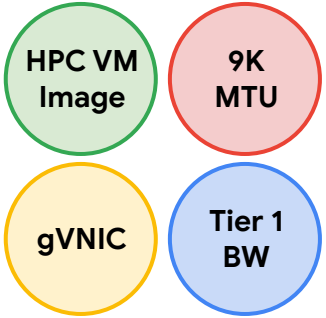
High Performance Compute

Google Cloud's HPC VMs have the **highest clock speeds** and **highest memory bandwidth** of any Google VM type. Choose Intel or AMD CPUs. VMs support **up to 16 NVIDIA GPUs**.



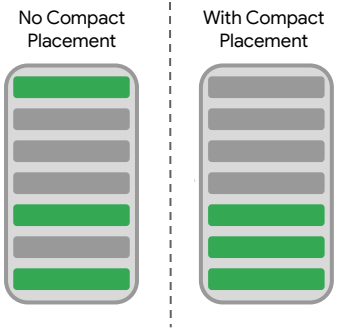
Virtual NUMA (vNUMA)

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. vNUMA is default on HPC VMs (C2*, A2).



Network Optimizations

Google's HPC VMs perform optimally with the best practice tunings in the HPC VM Image, as well as features like Tier 1 Bandwidth for 100Gbps, 9K MTU support, and gVNIC drivers.



Compact Placements

Compact placement policies put your VMs close together for low network latency between the VMs. Supports 100+ VMs per group. Supported by HPC VMs (C2*, N2*, A2).

Google Cloud

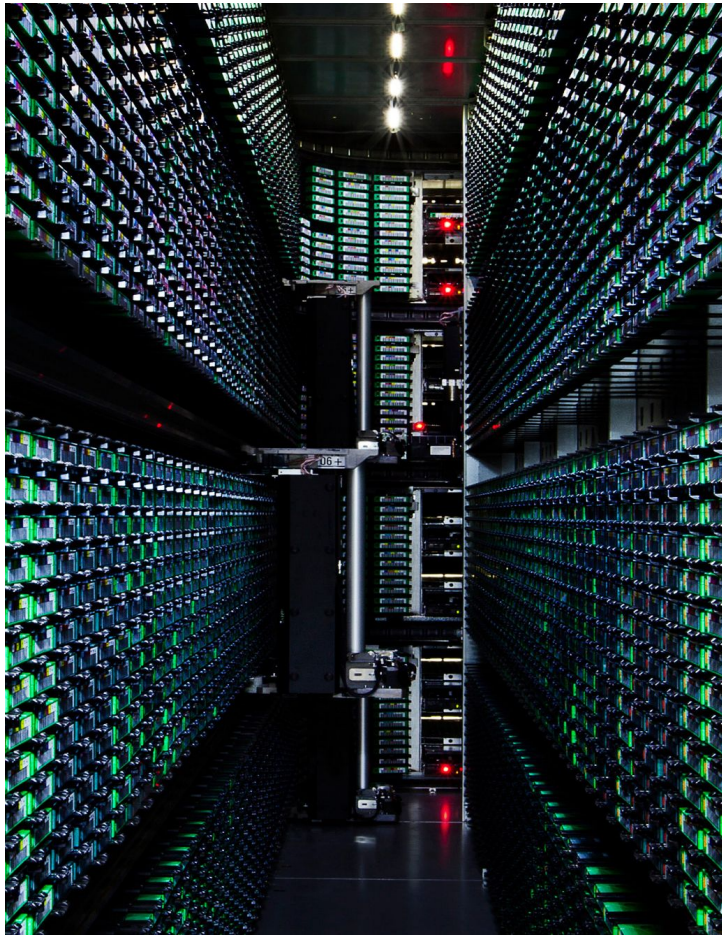
Google Compute Engine - GPUs

- Attached directly to the VM via PCIe x16, with NVLink and NVSwitch to achieve the best possible performance
- Per-second billing, Preemptible support (~70% off)
- First to market with NVIDIA A100, T4 GPUS

Google Cloud

Compute Engine - Bulk API

- **Large-scale Compute Engine creation API**
  - Deploy N identical instances
  - Regional deployment, zonal placement
  - Supports up to 1,000 instances
  - Supports all existing Compute Engine API features
- **Can speed up large-scale instance creation by 500%**
  - Single API call rather than a batched call, or sequence of calls
  - Capacity found together in a single operation
- Integrating into partner and open-source software (i.e. Slurm)



Google Cloud

Take advantage of configurable, short-lived instances, and discounts to save on cost

Custom Machine Types

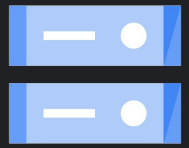
Choose your exact CPU/RAM ratio to match your workload

Committed use discounts

(up to 57% for most resource types) on longer term contracts

Spot VMs

Up to 91% cheaper, no bidding, no set time limit, all zones & regions



Storage

Google Cloud

HPC Storage on Google Cloud

Managed and open-source object, block, and file storage options

Google Cloud Storage
Exabyte-scale, feature-rich object storage
Automatically scaling throughput

Persistent Disk
SSD/HDD Persistent Disk
High-performance, replicated block storage

Local Storage
Local SSD (NVMe) for scratch and fast access
Physically attached to node via PCI

Cloud Filestore
Highly available, durable, POSIX-compliant shared storage
across tens of thousands of nodes

Partner, hybrid, and open-source
Storage solutions with NetApp, Dell, DDN, IBM, Lustre, and more
Move data to GCS with the Data Transfer Service and Appliance

Google Cloud

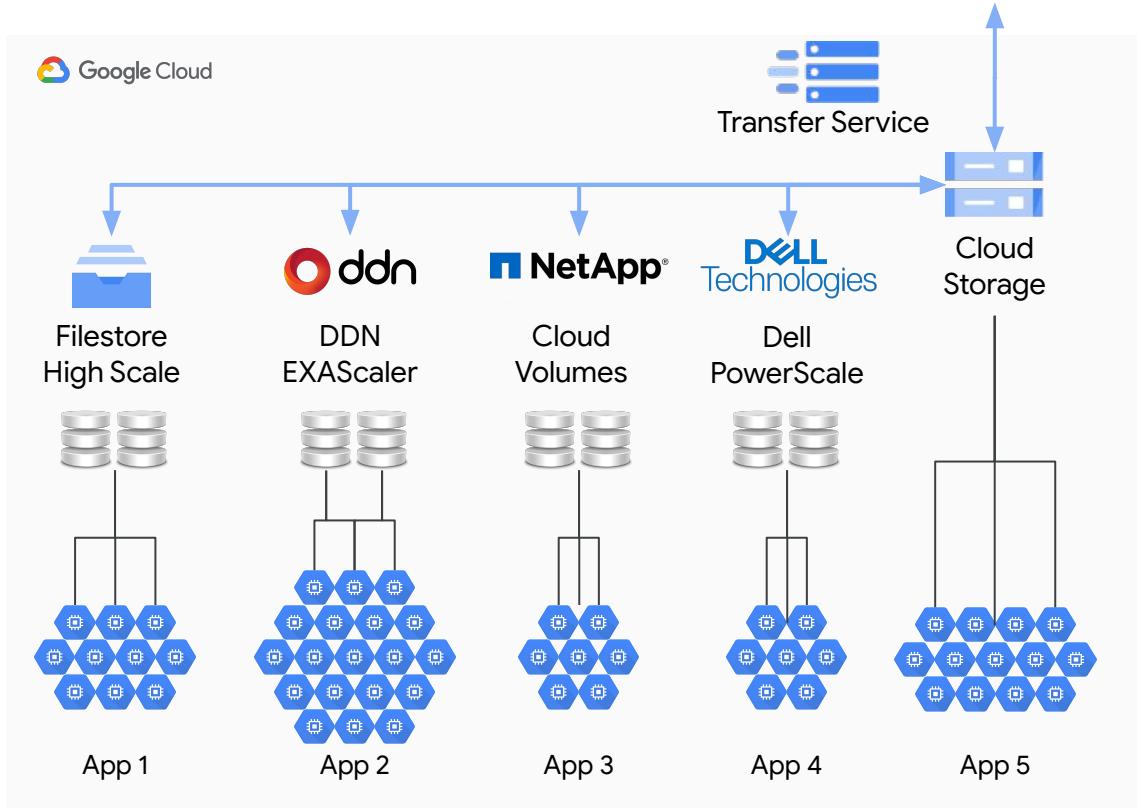
HPC Storage Building Blocks

Managed and open-source data storage and transfer options

Google is ready to build a hybrid, multi-site storage solution combining on-premises storage and Google HPC-ready storage options.

HPC-ready storage options on Google Cloud include:

- **Google's Cloud Storage**
  - Exascale object storage system, scales to Tb/s
- **Filestore High Scale**
  - Simple, scalable, managed NFS service
  - Up to 100's TBs, 10's GB/s throughput
- **NetApp Cloud Volumes**
  - Full featured NFS service, location-specific
  - NetApp FlexCache supported
- **Dell PowerScale**
  - Full featured NFS/SMB service, location-specific
- **DDN EXAScaler**
  - Lustre Parallel File System, Scales to 100+ GB/s
- **Solutions in development**
  - Intel DAOS and IBM Spectrum Scale (GPFS)
- **Transfer Service**
  - Data movement service for file and object storage
  - Available as software or hardware appliance

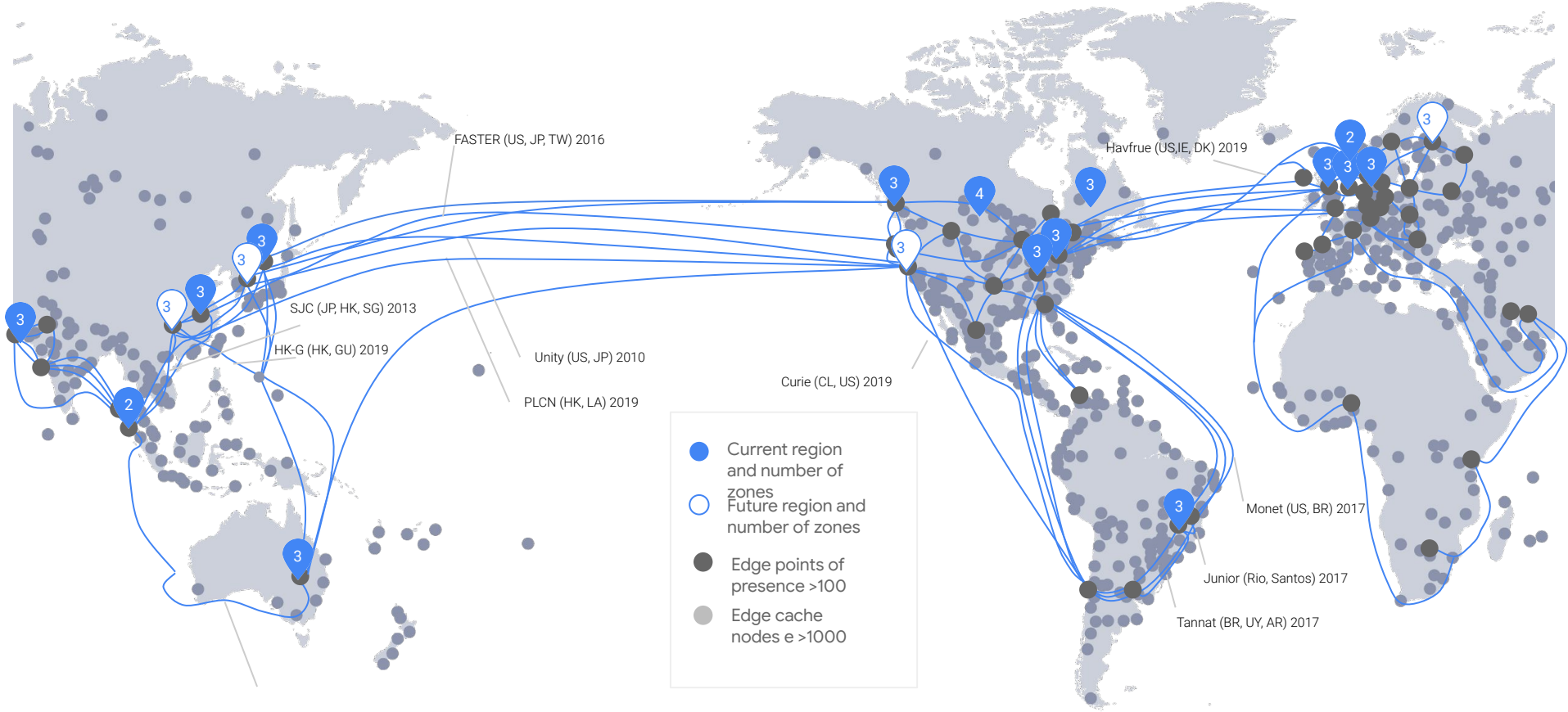


Network

Google Cloud

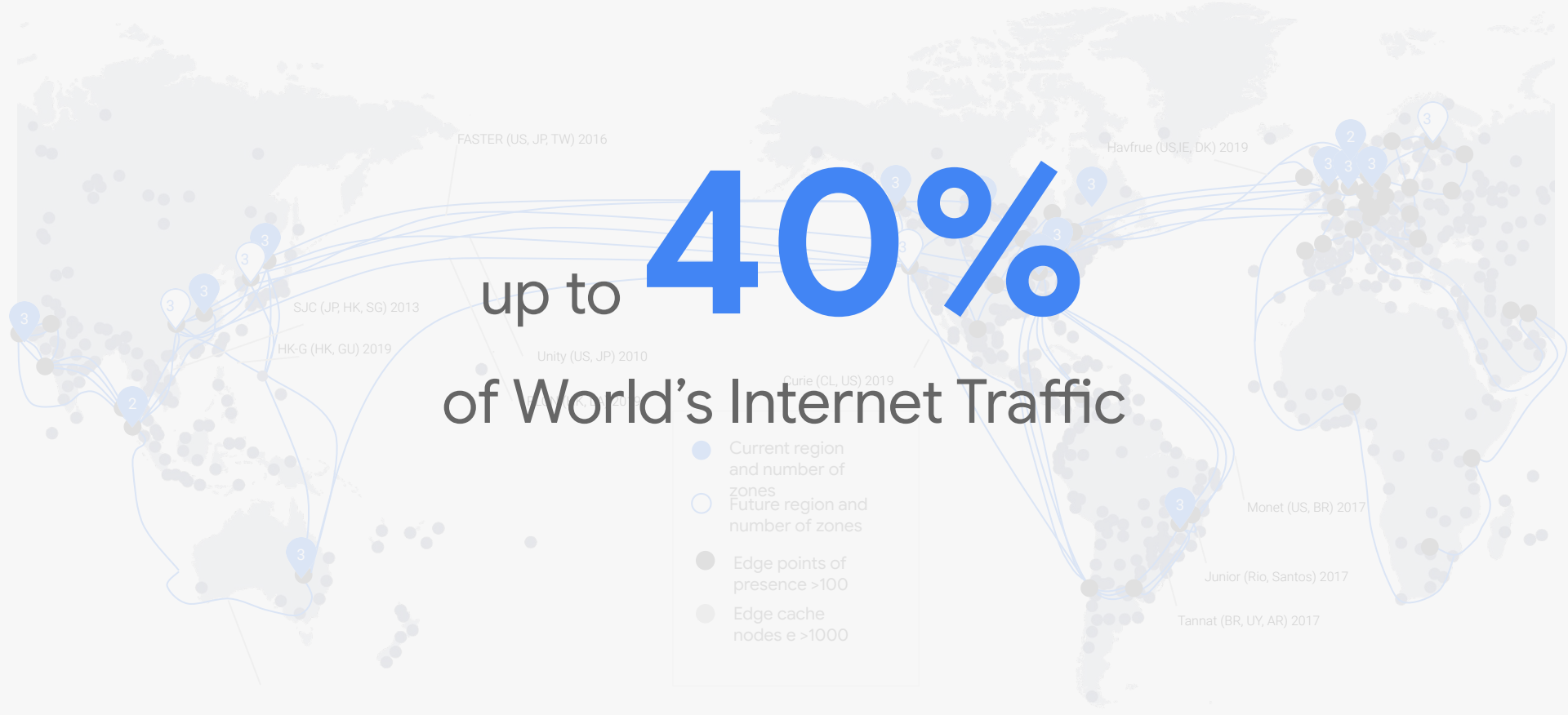
Global network infrastructure

The largest cloud network: 100,000s of miles of fiber optic cable, 8 subsea cables
More edge and peering points than any public cloud



Global network infrastructure

The largest cloud network: 100,000s of miles of fiber optic cable, 8 subsea cables
More edge and peering points than any public cloud

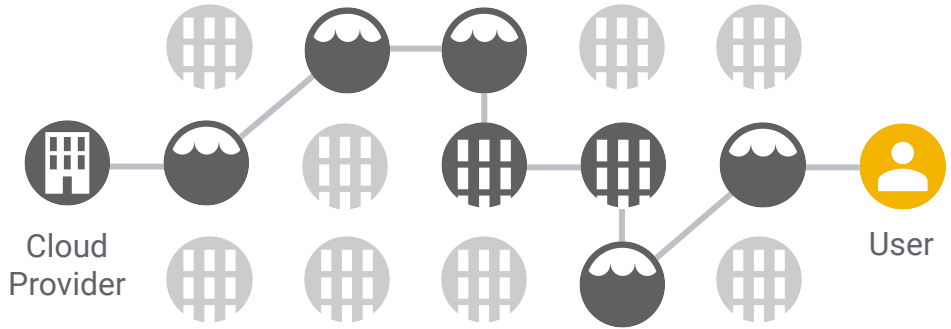


up to **40%**

of World's Internet Traffic

Google Cloud

The network matters.

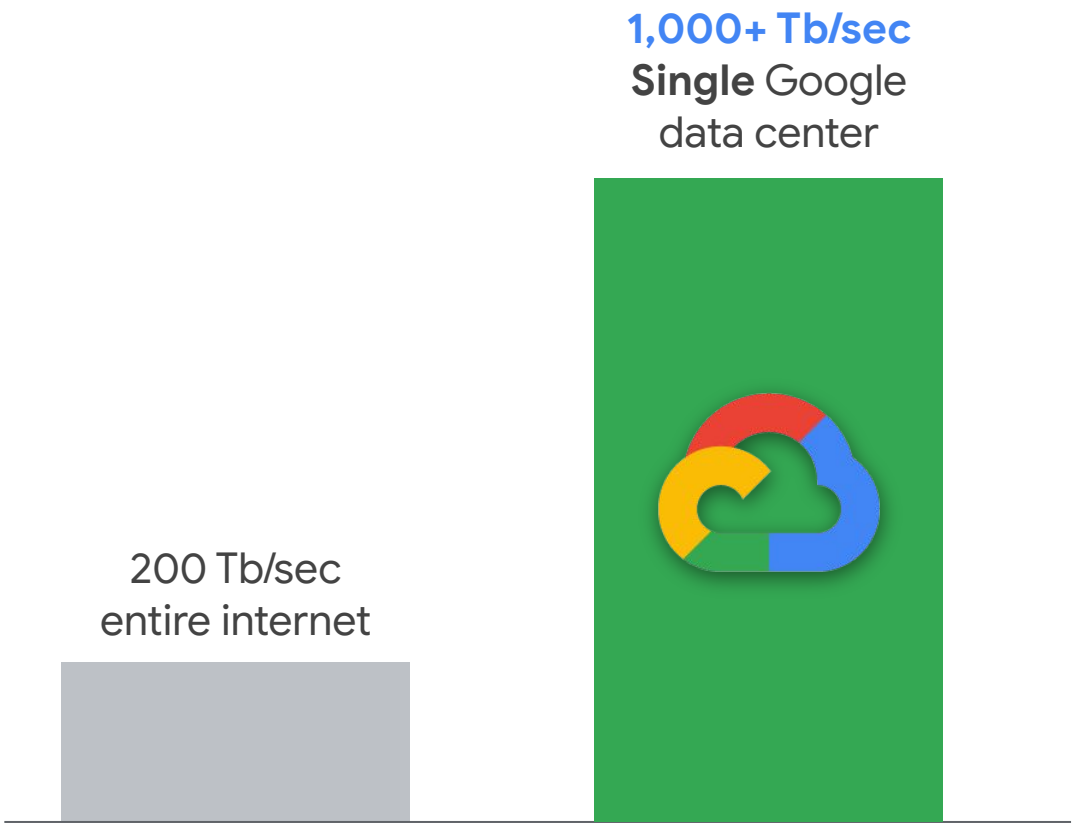


Typical cloud provider

Google Cloud

Google Cloud

Bisectional bandwidth



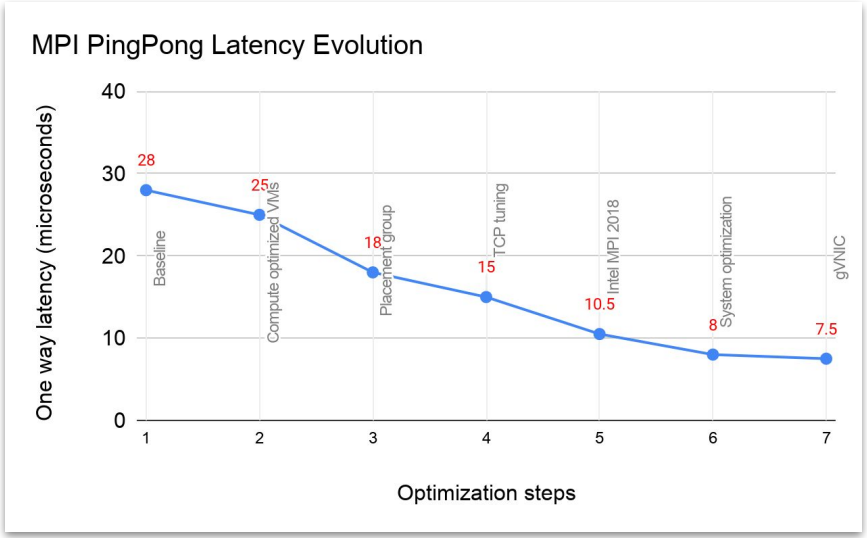
Google Cloud

https://cloudplatform.googleblog.com/2015/06/A-Look-Inside-Googles-Data-Center-Networks.html

HPC Networking on Google Cloud

Scalable, high-bandwidth, low-latency VM networking

- **Scalable Bandwidth**
  - 2 Gbps per vCPU
  - Up to **32 Gbps** per VM by default
  - **100 Gbps** with **Advanced Networking**
- **Low Latency**
  - Predictable, low latency (~10 µs average)
- **Tuning & Optimization**
  - **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
  - **9K MTU** (Jumbo Frames) in preview
- 15,000 VMs per Virtual Private Cloud Network



Google Cloud

HPC Software and Partnerships

02

Google Cloud

HPC Tools supporting Google Cloud

A growing ecosystem of HPC ISV and SI Partners and Open-Source Software

HPC APPLICATIONS - HPC powered applications tuned to harness Google Cloud

Life Sciences

Manufacturing

Financial Services

Electronics Design Automation

Interactive Computing

INFRASTRUCTURE & WORKLOAD MANAGERS - Tools and platforms for job scheduling and cluster management

Workload Managers

HPC as a Service

Containers

STORAGE - High performance storage systems for HPC workloads

SYSTEMS INTEGRATION - Experienced partners to implement your toughest workloads

Google Cloud

Slurm Workload Manager

Google partnered with SchedMD to integrate the Slurm Workload Manager with GCP to harness the elasticity of Compute Engine

Three 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.
- **Burst to Cloud:** Dynamically create virtual machines to offload jobs from your on-premise cluster to Google Cloud. Leverages Cloud Auto-Scaling functionality.
- **Federate to Cloud:** Federate jobs between your on-premise Slurm cluster and your Google Cloud Slurm cluster(s).
- **Open Source on SchedMD's Github:** https://github.com/schedmd/slurm-gcp
- **Auto-Scaling Slurm Cluster Tutorial:** https://codelabs.developers.google.com/codelabs/hpc-slurm-on-gcp

Google Cloud

On-Premises, Hybrid, Connectivity

Configure Google Cloud's HPC resources several ways:

- Stand-alone, isolated from on-premises resources
- Mostly separate, with cloud resources accessing on-premises resources including licenses and data
- Fully hybrid with on-prem resources triggering or fully managing cloud resources, and a hybrid data strategy

(1) Google's Interconnect or Cloud VPN can secure connections between Google and on-premises, as seen in this architecture.

High Performance Computing Architecture

Three-tiers: interactive (2), management (3), and compute nodes (4). Depending on your configuration, your management nodes (3) and interactive nodes (2) can exist in the cloud, on-premises, or both. Cloud resources are monitored by the Ops Suite (5), including Monitoring and Logging for HPC resources. Data can be pre- or post-processed using Google Cloud's various data analytics and data processing tools (6).

Workload Manager

All major workload managers and schedulers support Google Cloud in both stand-alone and hybrid deployments, including:

- Schedulers: SchedMD Slurm, IBM LSF, Altair PBS Works (PBS Pro, Grid Engine), HTCondor, MOAB, TIBCO GridServer
- Platforms: Rescale, Atos Nimbix, Parallel Works, UberCloud, Omnibond CloudyCluster, AlcesFlight, RONIN, Terra
- Google Tools: HPC Toolkit, Cloud Batch

(7) Partitions can specify configurations for deployment (region/zone, scaling limits), hardware (GPUs, Spot VMs, local ssd), and software (image, storage mounts, access controls).

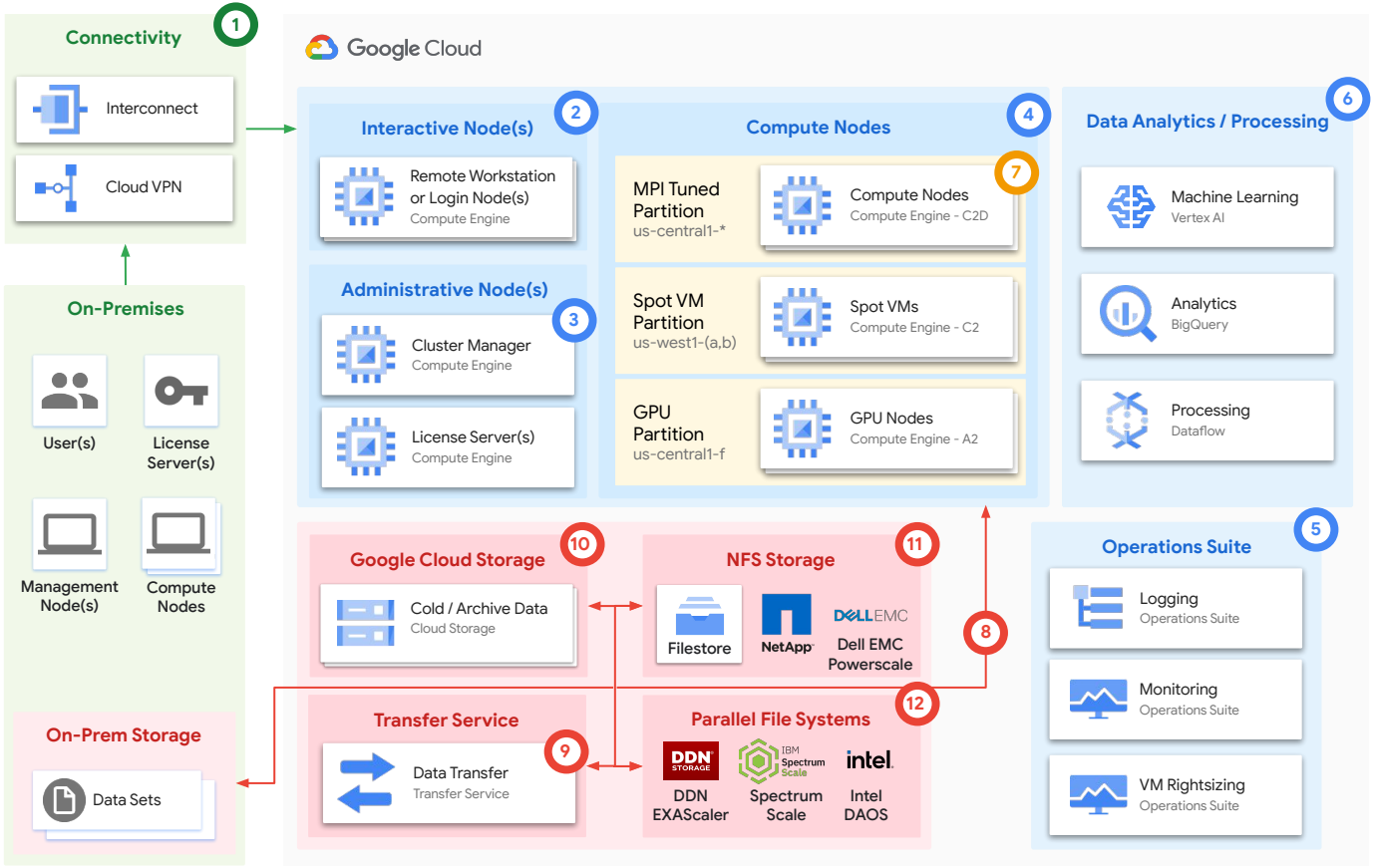
Data Storage

Managed and open-source data transfer and storage options:

- Directly from on-premises storage to VMs (8)
- Transferred using the Transfer Service to... (9)
- Google Cloud Storage (10)
- NFS Storage (managed or partner-provided) (11)
- Parallel File System (partner-provided) (12)

Open, Standards-Based Architecture for Cloud HPC

Intel HPC Platform Specification Compliant



Benefits of HPC VM Image

Quickly create HPC-ready VMs Out of box

- *Always stay up-to-date* with the latest GCP updates for tightly coupled workloads
- *No need to manually tune* MPI performance, no need for VM reboots

Tunings to unblock tightly coupled HPC workloads

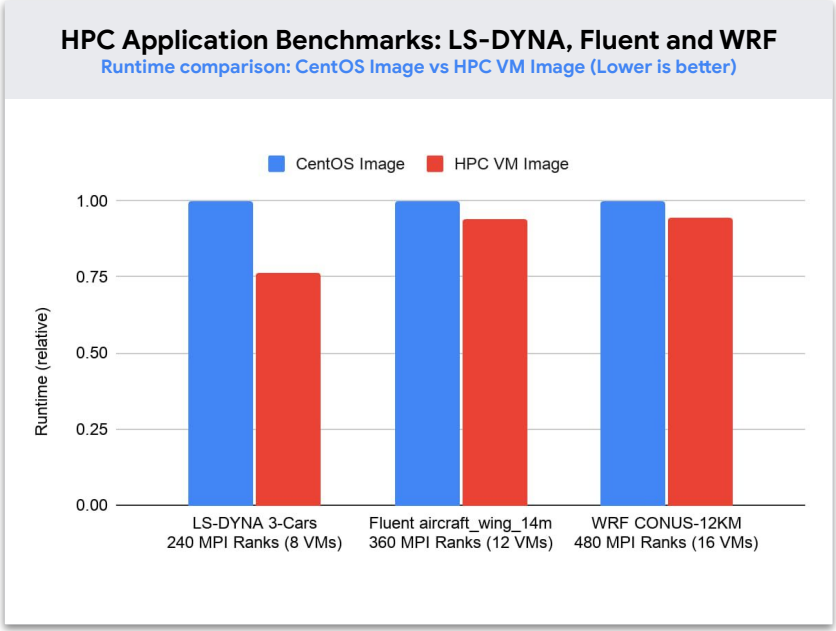
- Tunings and optimizations to *reduce latency for small messages*
- Will benefit applications which heavily depend on collective communications

Consistent Performance, Improved Usability

- Achieve *consistent, reproducible application-level performance*
- Easier HPC *cluster setup and maintenance* for HPC system administrators

HPC VM Image

- **CentOS 7 based VM Image**
- **Tunings and Optimizations Included**
  - Adjust user limits on system resources
  - Increase tcp *mem settings
  - Use the network-latency profile
  - Disable Linux firewalls
  - Disable SELinux
  - Intel MPI collective tunings
  - (Optional) Disable Spectre/Meltdown patches
- Available as a stand-alone image, in the Marketplace, or as individual tunings you can apply to your own images
- Integrated with HPC Partners (i.e. Slurm, CloudyCluster)



https://cloud.google.com/blog/topics/hpc/introducing-hpc-vm-images

Proprietary + Confidential

Introducing the Cloud HPC Toolkit

Easily create turnkey HPC environments

- Easily create turnkey HPC environments and get the best performance out-of-the-box
- Start with verified cluster blueprints and stay up to date with GCP best practices

Configurable, extensible and open-source

- Based on standard tech stack, and allows a broad set of cluster customizations
- Open source - available for customers and solution providers to add new features

Supports analytics via Cloud Monitoring

- Built-in labeling functionality makes it easy to track resources with Cloud Monitoring
- Optional custom HPC labeling available to get insights on cluster performance

Community and Getting Started

Google Cloud

Our Commitment to Sustainability

100% Renewable
Since 2017, Google has matched all of its energy consumption with purchases of renewable energy

5.5 GigaWatts
Global renewable energy under contract by Google today

Carbon Neutral for 13 Years
Google has been carbon neutral since 2007

Carbon Free by 2030
has committed to achieving 100% 24/7 carbon-free operations by 2030.

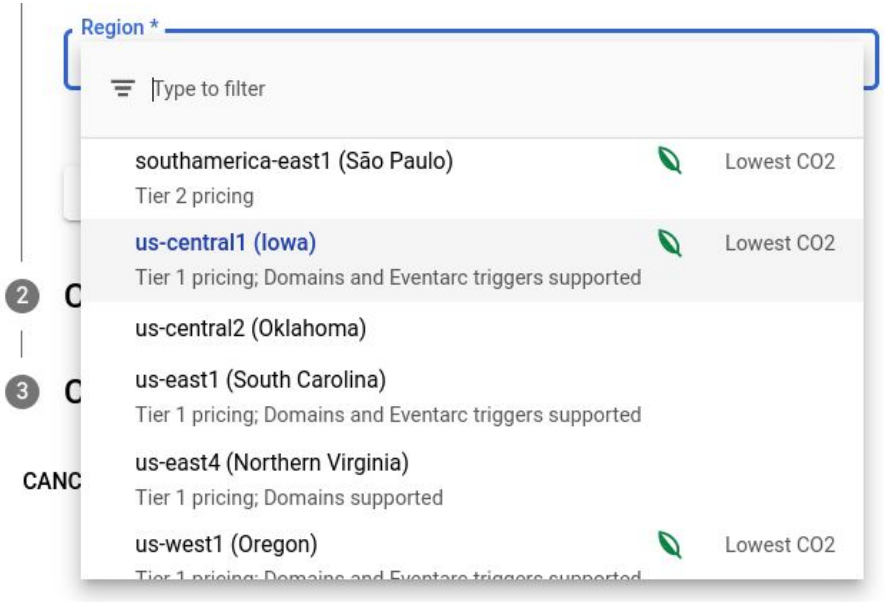
Google Cloud

Console region pickers show carbon info

Surface carbon-related info in context of Cloud Console.

Incentivise developers to pick more sustainable regions.

Fun fact: there is often a correlation between sustainable regions and lower prices (greenest is often the cheapest)



Google Cloud

Demo: Carbon information in Cloud Run region picker

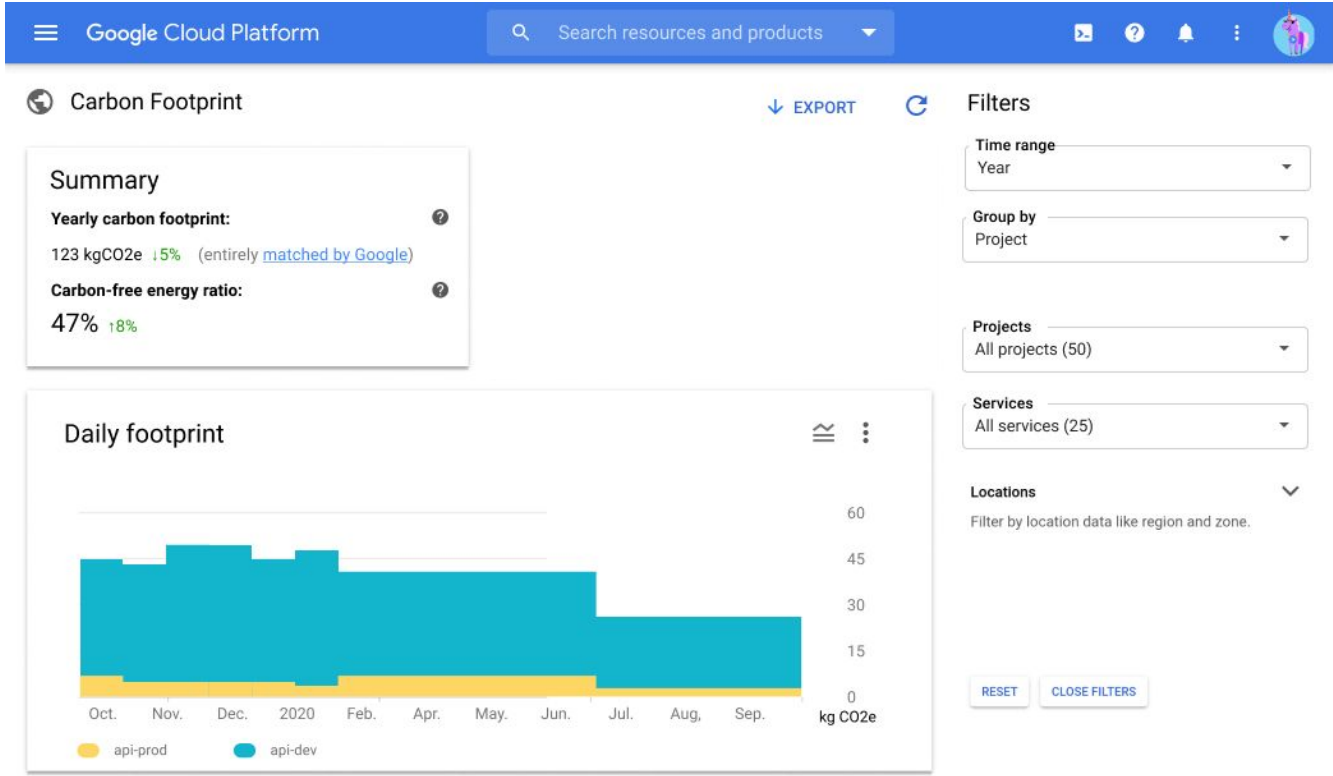
Per-customer carbon footprint

Organization-wide view.

Data broken down by:

- project
- region
- product
- timeframe

Data export to BigQuery.



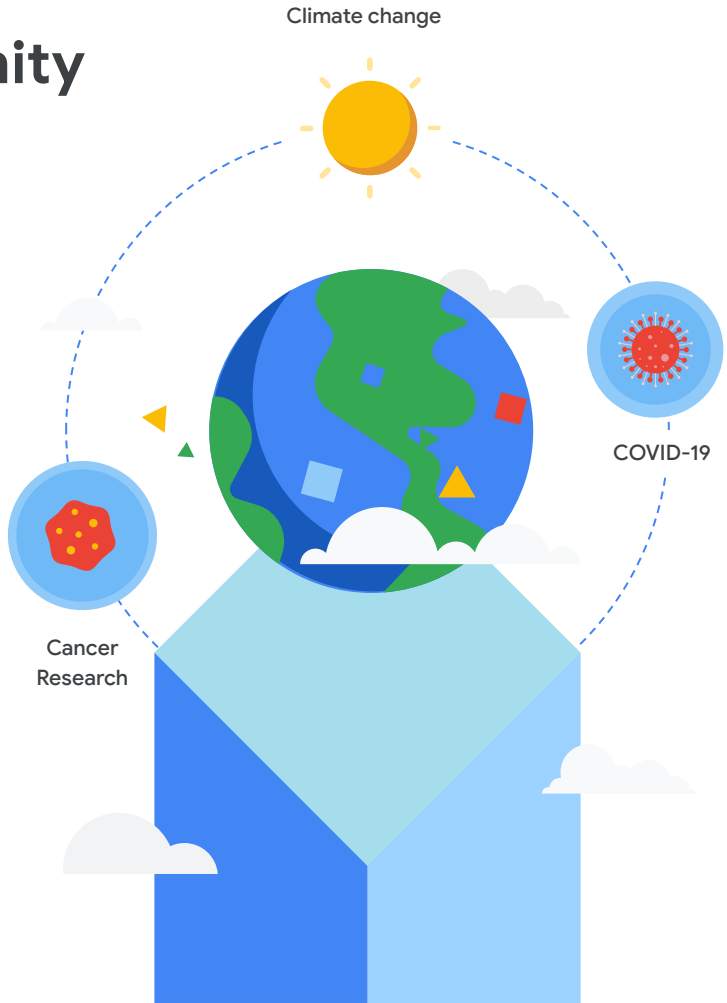
Google Cloud

Supporting the Research Community

Google aims to enable researchers to use our tools and technology to investigate some of the world's biggest challenges such as cancer, climate change, and most recently COVID-19.

We offer several programs to support research being done in the cloud:

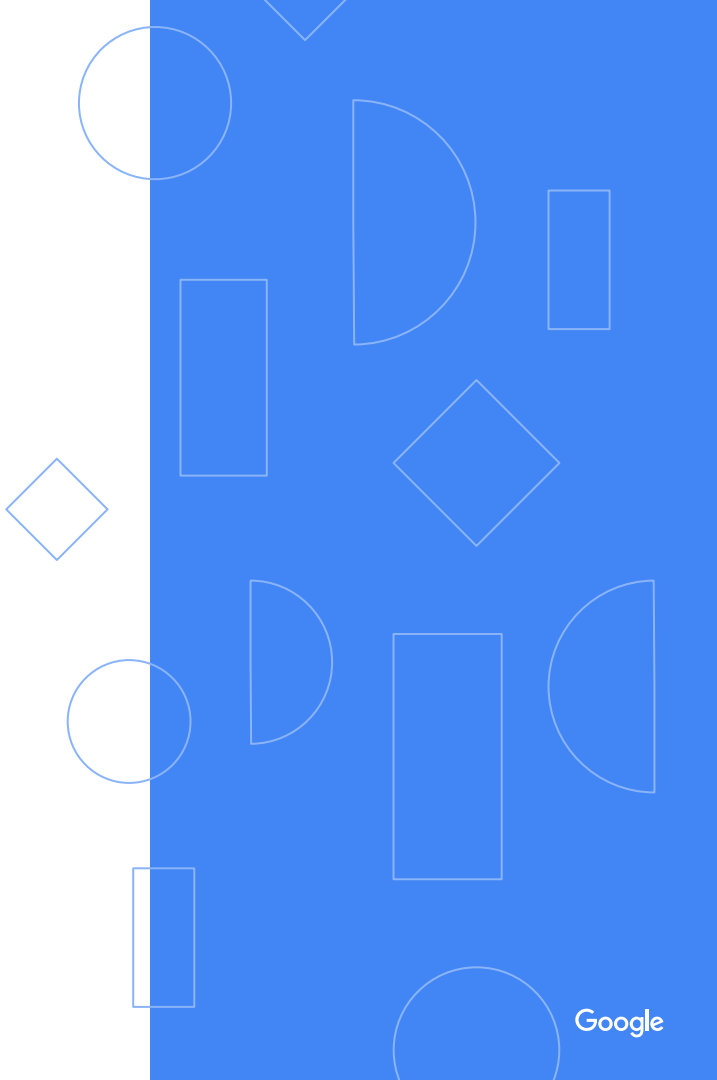
- National Institutes of Health (NIH)'s STRIDES Program
- NIH's CloudBank
- Google Cloud Research Innovator's Program
- Google Cloud Public Datasets Program
- Google Cloud Research Credits Program
- Google Cloud Academic Credits Program



Google Cloud

Getting Started

- Learn More at: https://cloud.google.com/hpc
- Review our Case Studies
- Step-by-Step guidance from the Architecture Center
- Schedule an HPC Day hands-on workshop with Google Cloud HPC SMEs.



Google

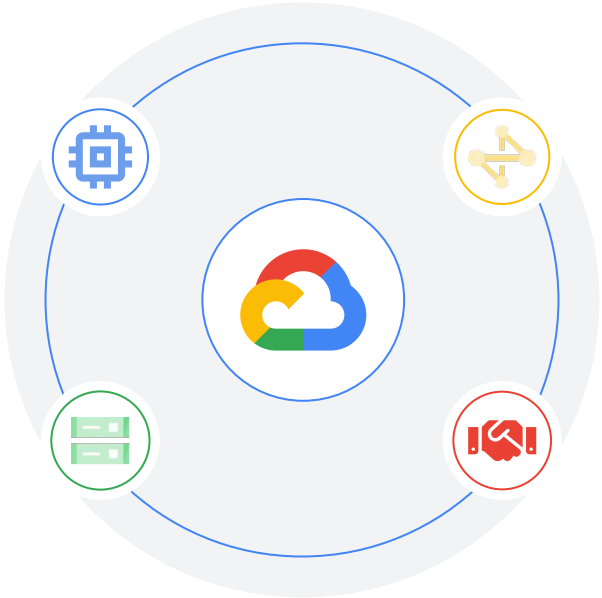
High Performance Computing
on Google Cloud

Compute

Google Compute Engine's VMs boot in seconds, are built for consistently high performance, and have security built-in.

Storage

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



Network

Google's high performance private network connects VMs with high throughput, low latency interconnects.

HPC Software

Google Cloud offers native HPC tooling, and supports a broad portfolio of HPC software from our HPC Partners and Open-Source projects.

Thank you.

https://cloud.google.com/hpc

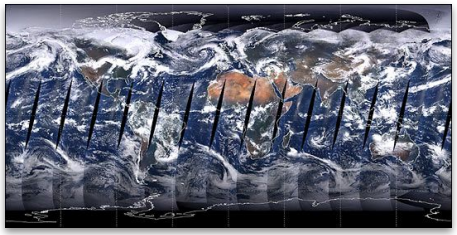
Google Cloud

Proprietary + Confidential

Google Earth Engine is a differentiated **spatial data and analytics platform** with a long history in enabling environmental and social impact

Data Catalog

The world's largest archive of open Earth data at your fingertips.

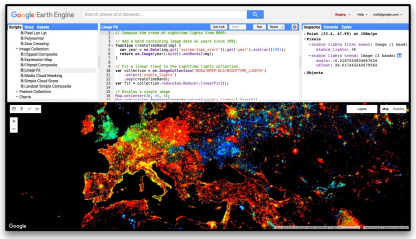


700+ curated geospatial datasets, including near-real-time satellite imagery.

+

Computation Platform

A powerful tool to analyze and visualize Earth data at scale.



Parallel processing for speed and scale, with machine learning built in.

+

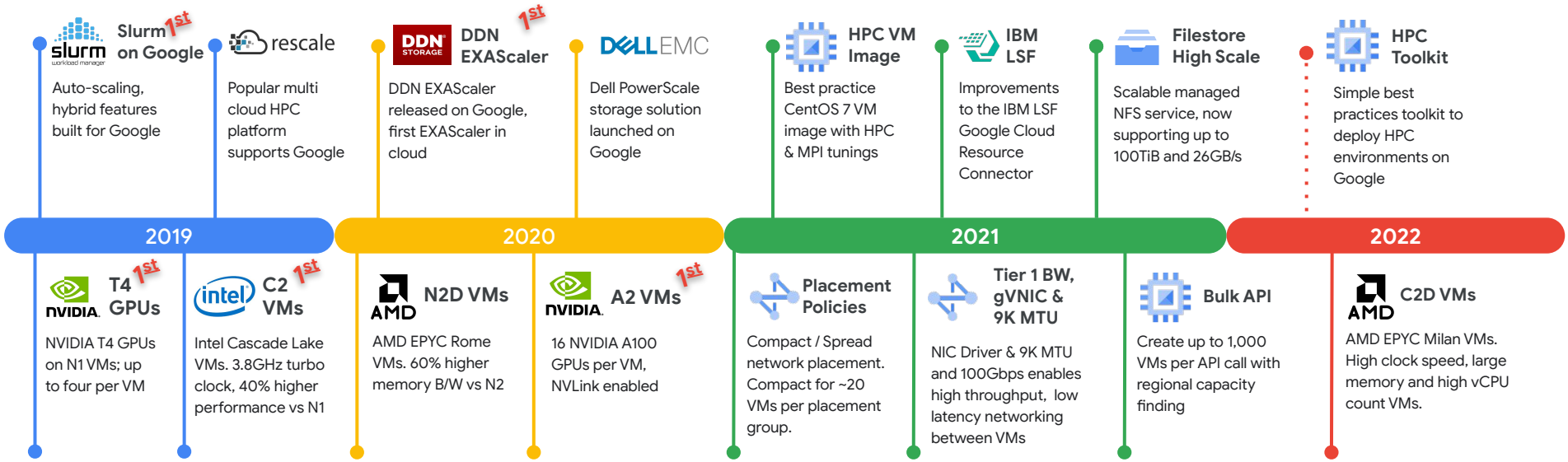
Collaborative Ecosystem

50,000 sustainability-focused MAUs (and growing).

A rich user community focused on sustainability, social and environmental impact

Investing in HPC Infrastructure and Software

1st = First in cloud



* In Preview

Legend
Available
In Preview

DDN STORAGE + Google Cloud

#8 Filesystem and Top Lustre System on the IO-500

Build your own world-class Lustre filesystem with DDN EXAScaler in the GCP Marketplace, or deploy Open Source Lustre with our easy to use tools.

IO500

# ↑	BOF	INSTITUTION	SYSTEM	STORAGE VENDOR	FILE SYSTEM TYPE	CLIENT NODES	TOTAL CLIENT PROC.	SCORE ↑
1	ISC21	Pengcheng Laboratory	Pengcheng Cloudbrain-II on Atlas 900	Pengcheng	MadFS	512	36,864	36,850.37
2	ISC21	Intel	Endeavour	Intel	DAOS	10	1,440	1,859.56
3	ISC20	Intel	Wolf	Intel	DAOS	52	1,664	1,792.98
4	ISC21	Lenovo	Lenovo-Lenox	Lenovo	DAOS	36	3,456	988.99
5	SC19	WekaIO	WekaIO on AWS	WekaIO	WekaIO Matrix	345	8,625	938.95
6	ISC20	TACC	Frontera	Intel	DAOS	60	1,440	763.80
7	ISC21	National Supercomputer Center in GuangZhou	Venus2	National Supercomputer Center in GuangZhou	kapok	18	720	577.93
8	ISC21	Google Cloud	Google	DDN	Lustre	1,000	5,000	569.99
9	ISC20	Argonne National Laboratory	Presque	Argonne National Laboratory	DAOS	16	544	537.31
10	SC19	National Supercomputing Center in Changsha	Tianhe-2E	National University of Defense Technology	Lustre	480	5,280	453.68

IO500 ISC21 List
https://io500.org/

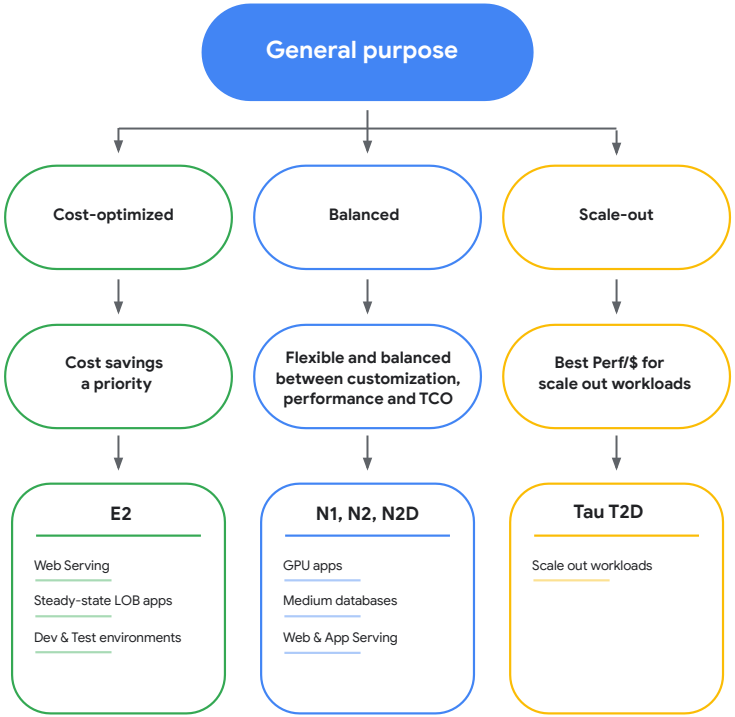
Google Cloud

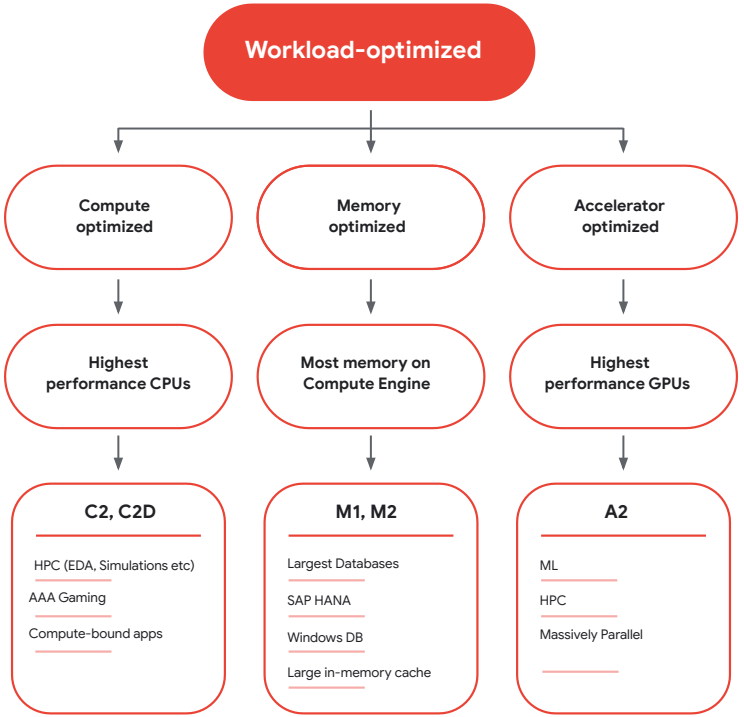
HPC Customers

Enterprise

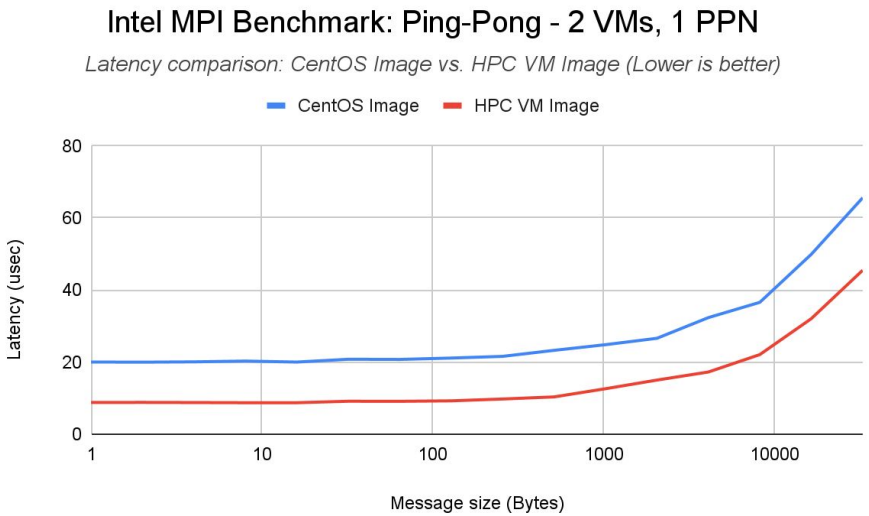
Higher Education

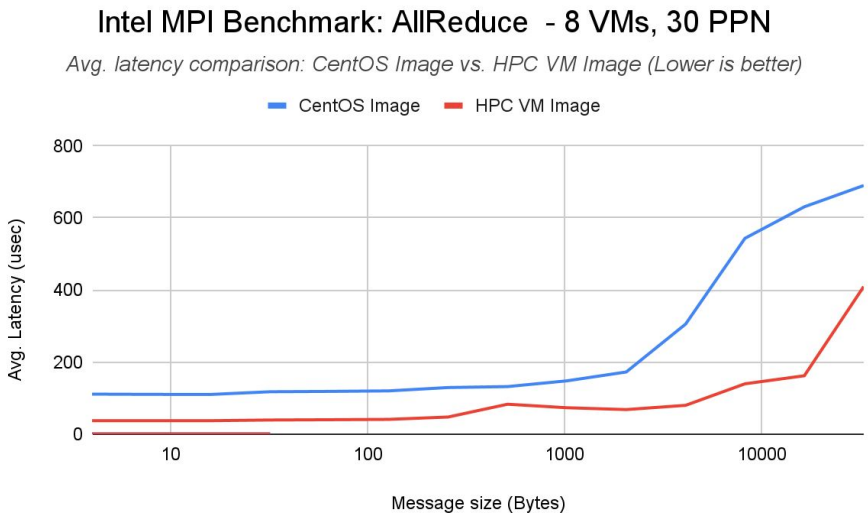
VM families for all workloads





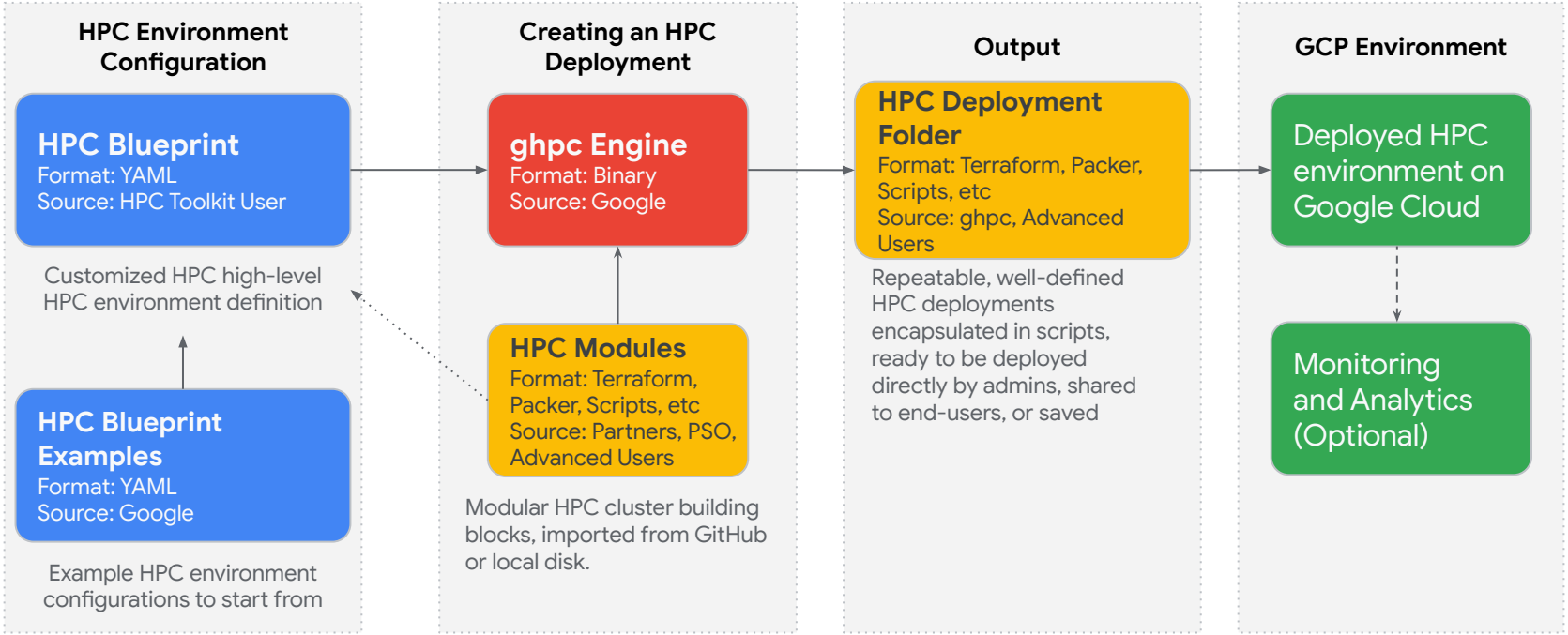
Intel MPI Benchmarks using HPC VM Image



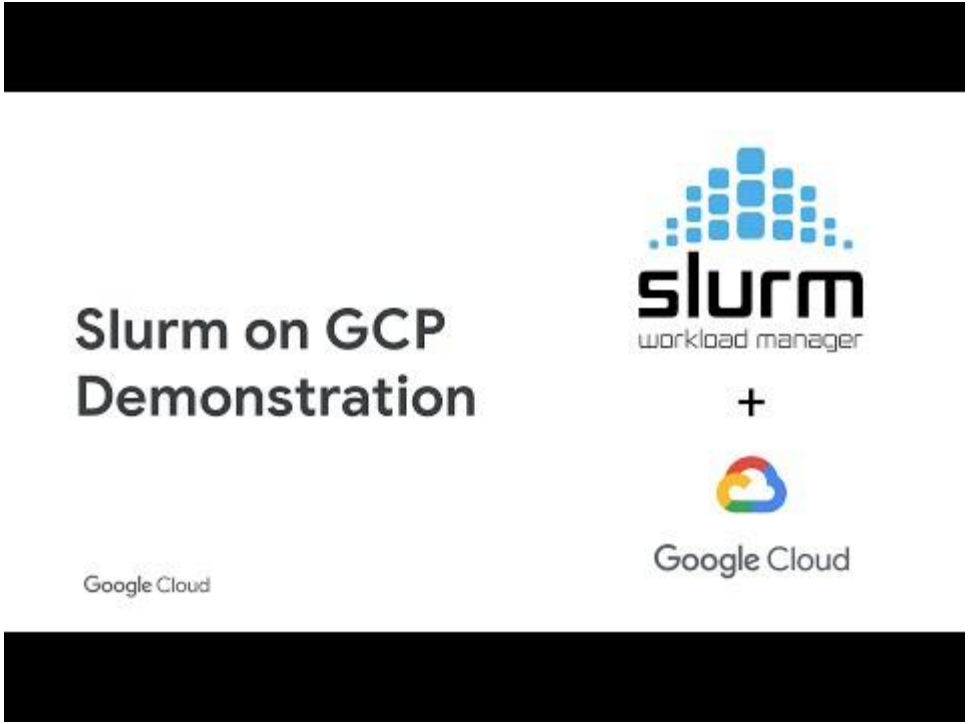


Proprietary + Confidential

HPC Toolkit Architecture



Slurm Auto-Scaling Demo



Google Cloud

Descartes Labs

Industry: Technology, Agriculture, Forestry & Fishing
Country: United States
In partnership with:

intel

Challenge

To power its satellite imagery platform, the **machine learning intelligence developer** sought a solution that could provide analytics processing alongside detailed global satellite imagery at scale.

Data analytics: Developing global insights

Google Earth Engine works alongside BigQuery, Compute Engine and other Google solutions to support the Descartes platform. Descartes geospatial analysis uses Google Cloud solutions to realize insights including crop and global water supply trends.

Accelerates time to market for research results by more than six months with Google Cloud Platform	Able to **process petabytes of data in hours** while avoiding large capital expenditures	Improves **speed and accuracy** of crop yield data

"With Google Cloud Platform, we don't worry about whether the compute, network, or storage can scale. We can focus on improving models and analyzing larger datasets for better forecasts."

Tim Kelton, Co-founder and Cloud Architect, Descartes Labs

Google Cloud