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HPC in the City: *St. Louis* HACKATHON



Google and CloudyCluster Training



Join the HPC in the
City Discord using
this QR Code!



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TEXAS ADVANCED COMPUTING CENTER



HPC
in the
City: *St. Louis* HACKATHON



St. Louis, MO | science & beyond.

**Google and
CloudyCluster
Training**

Agenda

- Introductions
- Hackathon Objective
- Deliverables and Resources
- General Information
- Google Cloud Platform
- Cloudfcluster



Presenter: Je'aime Powell

Organizers



Alex Nolte - *University of Tartu*
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Boyd Wilson - *Omnibond*
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Amy Cannon - *Omnibond*
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Je'aime Powell - *TACC*
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Linda Hayden - *ECSU*
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The Objective of HPC in the City: St. Louis

The hackathon aims to harness the resources, skills, and knowledge found in the HPC community in an effort to provide applied exposure towards students from 2-4 year post-secondary educational institutions. In short, the hackathon will provide HPC skills and training while targeting problems that directly affect the participants.

- Develop knowledge about solutions to identified issues affecting St. Louis through application of data analysis/presentation or management.

Student Outcomes

- Increased familiarity with data science in the cloud
- Experience collaborative software engineering
- Develop professional communication skills

Student Deliverables and Resources

Deliverables:

- **Source code Including Comments**
- **PDF of presentation**
 - Team members with pictures
 - Use of HPC technology in the project
 - Regional (St. Louis) implications of the project
- **Github Repository Link**
 - README.md with project description

Resources:

- **Google Cloud (Provided Credits)**
- **Cloudy Cluster**
- **Most Commonly Used**
 - Python
 - Jupyter Notebooks
 - Node.Js (JavaScript)
 - Repl.it (Collaborative Environment)
 - HTML
- **Discord**
<https://discord.com/invite/rSXasYKDwE>



Join the HPCHack
Discord using this
QR Code!

General Information (the 3 T's)

- **Teams**

- 4-5 Students
- 1 Primary Mentor
- 1 Specialist/Staff

- **Time**

- November 4th - 8th
 - 11/4@~6pm ET Event Start
 - Team formation
 - 11/[5-8] @ 11 ET & 6pm ET- Checkins
 - 11/8@6pm ET-Final Presentations

- **Topic Examples**

- Data Analysis of COVID 19
- Economic disparities and their effects on college participation
- Genomics, Molecular Dynamics, or Weather Modeling in the Cloud.
- Social Justice
- AI-based Crowd Status
- Public Data Management
- Graduation Rates
- Broadband Access
- Insurance vs. Public Health Resilience

HPC Resource Platforms





cloudyclusterTM

Turn-Key Cloud HPC

gcp.cloudycluster.com

By Omnibond

Omnibond - Introduction

Leadership Team

- Former COO at NCSA
- CIO at Purdue and Clemson Universities
- Sw CTO - Clemson University
- Director Computing Engineering School
Miami Ohio
- Consultant to Tribal Colleges and Minority
Serving Institutions on cyberinfrastructure
- Founded ACI-REF <http://www.aciref.org>
and CaRCC <http://carcc.org>
(Emphasize the human element)

Software Products

- Cloud Orchestration - **CloudyCluster**
- Computer Vision & AI based **TrafficVision**
analytics system.
- Parallel File System - **OrangeFS** included
upstream in the Linux Kernel
- Identity Management - **Identity Manager
Connectors**
 - products installed in thousands of
customers worldwide

Google Cloud Console

i Google Cloud Next '21 is live. Join us now at g.co/cloudnext. [DISMISS](#)

Project info

Project name
CloudyClusterFirebaseDev

Project ID
cloudyclusterfirebase-dev

Project number
944159813764

[ADD PEOPLE TO THIS PROJECT](#)

[Go to project settings](#)

Resources

- Compute Engine**
11 instances
- Storage**
40 buckets
- Cloud Functions**
14 functions

Trace

URI	50th	90th
/_ah/push-...		
/		
/owa/auth...		

Compute Engine

CPU (%)

Instance/cpu/utilization: 4.75%

[Go to Compute Engine](#)

API APIs

Requests (requests/sec)

Requests: 0.000/s

Google Cloud Platform status

All services normal

[Go to Cloud status dashboard](#)

Billing

Estimated charges USD \$120.03
For the billing period Oct 1 - 14, 2021

[Take a tour of billing](#)

[View detailed charges](#)

Monitoring

- [Create my dashboard](#)
- [Set up alerting policies](#)
- [Create uptime checks](#)
- [View all dashboards](#)

[Go to Monitoring](#)

API Error Reporting



Turn-Key HPC with CloudyCluster

CloudyCluster = Automated Cloud CyberInfrastructure

- Automated Deployment of fully functioning HPC/HTC environment (Complete with VPC, firewall config, scheduler, login, parallel & object storage)
- Provides users a familiar HPC & HTC experience to on-prem
- Over 300 HPC, HTC, and AI packages and libraries pre-configured
- Job scripts determine instances used (Standard, Preemptible, GPU)
- Slurm or Torque fronted by the powerful CCQ meta-scheduler
- Parallel and Object storage Options
- Operates in the customer's own GCP account (eliminating 3rd party BAAs)
- HPC / HTC job integration with GCP Billing Labels
- Automatically leverages GCP Placement Policies for jobs using Supported (C2) Instances



Self-Service Elastic HPC & HTC

1. Cloud HPC orchestration

You Create a fully operational & secure computation cluster in minutes, complete with:

Encrypted Storage: GCS, OrangeFS on PD

Compute: Job Driven Elastic Compute through CCQ

Scheduler: Torque & SLURM with the CCQ Meta-Scheduler

Includes over 300 packages and libraries used in HPC including:

HPC Libraries:

Boost, Cuda Toolkit, Docker, FFTW, FLTK, GCC, Gengetopt, GRIB2, GSL, Hadoop, HDF5, ImageMagick, JasPer, mpich, NetCDF, NumPy, Octave, OpenCV, OpenMPI, PROJ, R, Rmpi, SciPy, SWIG, WGRIB, UDUNITS, .NET Core, Singularity, Queue, Picard, and xrootd

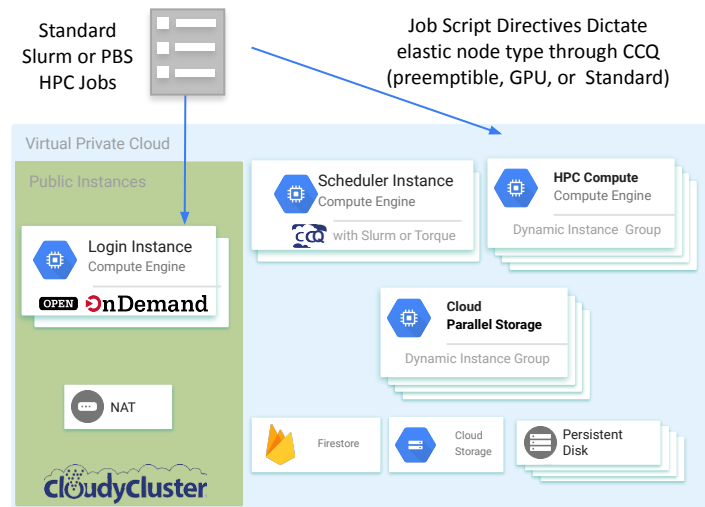
HPC Software:

Ambertools, ANN, ATLAS, BLAS, Blast, Blender, Burrows-Wheeler Aligner, CESM, GROMACS, JupyterLab, LAMMPS, NCAR, NCL, NCO, nwchem, OpenFoam, papi, paraview, Quantum Espresso, SAMtools, WRF, Galaxy, Vtk, Suz, Dakota, and Gatk

ML Software:

Mpack, NuPIC, Octave, OpenCV, PICARD, Queue, Scikit-learn, Tensorflow and Theano

Customization: You can easily add your own software to a custom Image.



Consumption, Deployment & Engagement

CloudyCluster can be launched easily from the GCP Marketplace:

- Launch easily from the GCP Console
- Pricing is about 5% of on-demand costs
- Can be sold as a subscription for select customers

The CloudyCluster Team Can Help with:

- HPC & HTC Discussions (Consulting and Pre-Sales)
 - Workloads that work well in the Cloud
 - Migrating HPC & HTC Jobs that can run in the cloud and on premises
 - Cloud HPC Cost Estimates
 - Proof of Concept (POC) workflow
- Additional Services available for tighter campus integration



Google Cloud Platform CloudyClusterFirebaseDev Search

New CloudyCluster deployment

Deployment name: cloudycluster-1

Zone: us-central1-f

Machine type: 1 vCPU 3.75 GB memory Customize

Previously created SA: SERVICE_ACCOUNT_NAME (from script)

Service Account API Permissions: Allow CloudyCluster to use the Scopes of the provided SA

Create a custom CloudyCluster image: Create a custom image

Boot Disk: Boot disk type: SSD Persistent Disk; Boot disk size in GB: 45

Networking: Network: default; Subnetwork: default (10.128.0.0/20)

Firewall: Allow HTTP traffic; Allow HTTPS traffic

Deploy

CloudyCluster overview
Solution provided by Omnibond

Solution trial
This trial lets you try out this solution, using the default configuration, without paying for license fees up to \$500.00, or for a maximum of 60 days, whichever comes earlier. During the trial, you will be billed for license fees and then credited at the same time for those license fees up to \$500.00. Additionally, you will still be billed for any applicable infrastructure usage charges during the trial.
When your trial use exceeds \$500.00 in license fees or 60 days, whichever comes earlier, you will be charged license fees unless you stop or delete the deployment. You may cancel the trial at any time by deleting the trial deployment prior to the end of the trial.
By deploying this solution, you accept and agree to the terms above.

\$33.09 per month estimated
Effective hourly rate \$0.045 (730 hours per month)
Details

Software

Operating System	CentOS (7)
Software	CloudyCluster (2.0.1)

Terms of Service
By deploying the software or accessing the service you are agreeing to comply with the Omnibond terms of service, GCP Marketplace terms of service and the terms of applicable open source software licenses bundled with the software or service. Please review these terms and licenses carefully for details about any obligations you may have related to the software or service. To the limited extent an open source software license related to the software or service expressly supersedes the GCP Marketplace Terms of Service, that open source software license governs your use of that software or service.
By using this product, you understand that certain account and usage information may be shared with Omnibond for the purposes of sales attribution, performance analysis, and support.
Google is providing this software or service "as-is" and any support for this software or service will be provided by Omnibond under their terms of service.

Online Training - Qwiklabs

Qwiklabs

Here is the link to apply for credits with qwiklabs:

<https://www.cloudskillsboost.google/focuses/21221?parent=catalog>

Here is the link to the CloudyCluster qwiklab:

https://edu.google.com/programs/credits/training/?modal_active=none

Start Lab

01:30:00

Student Resources

- ↓ Job Scripts
- ↓ Using the CCQ Meta-scheduler
- ↓ Blog Articles
- ☑ Behind the Scenes Architecture of CloudyCluster v3 on GCP

Omnibond: Creating an HPC Environment in Google Cloud with CloudyCluster

1 hour 30 minutes 5 Credits ☆☆☆☆☆

This lab was developed with our partner, [Omnibond](#). Your personal information may be shared with Omnibond, the lab sponsor, if you have opted-in to receive product updates, announcements, and offers in your Account Profile.

GSP862

Overview

Setup and Requirements

Google Cloud Project Setup

Launch CloudyCluster

Configure the Control Instance

Behind the Scenes

HPC Job Execution

Deleting CloudyCluster

Congratulations!

HPC Workloads for Google Cloud

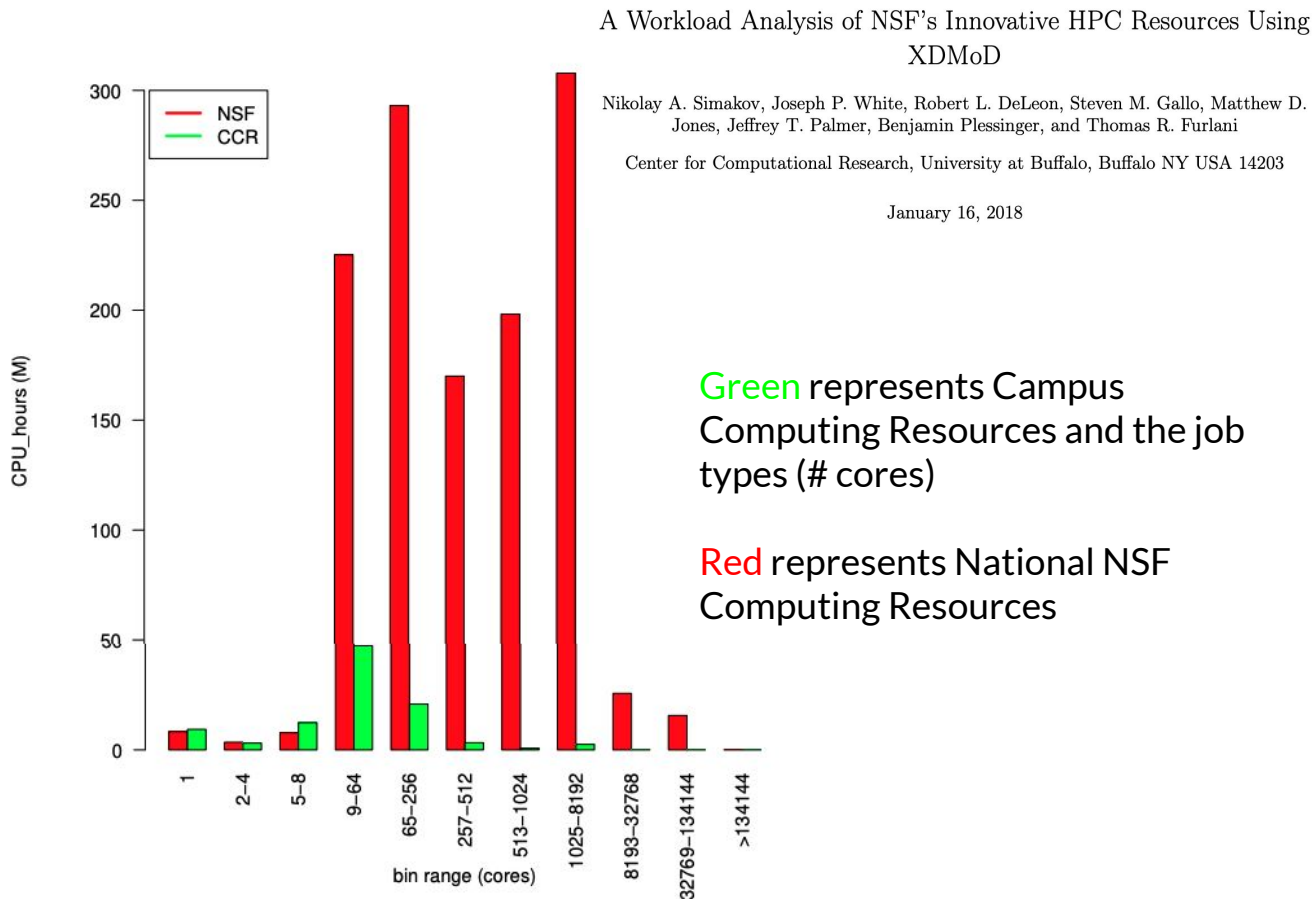


If you look at the Campus resources a majority (>90%) of the jobs will run on <9 instances (given 30 cores per instance).

The MPI latency between <9 instances is only impactful on a very small number of job types.

A majority of workloads run on a campus cluster will be supported in GCP

The larger NSF resources require more investigation



Google Cost Comparison

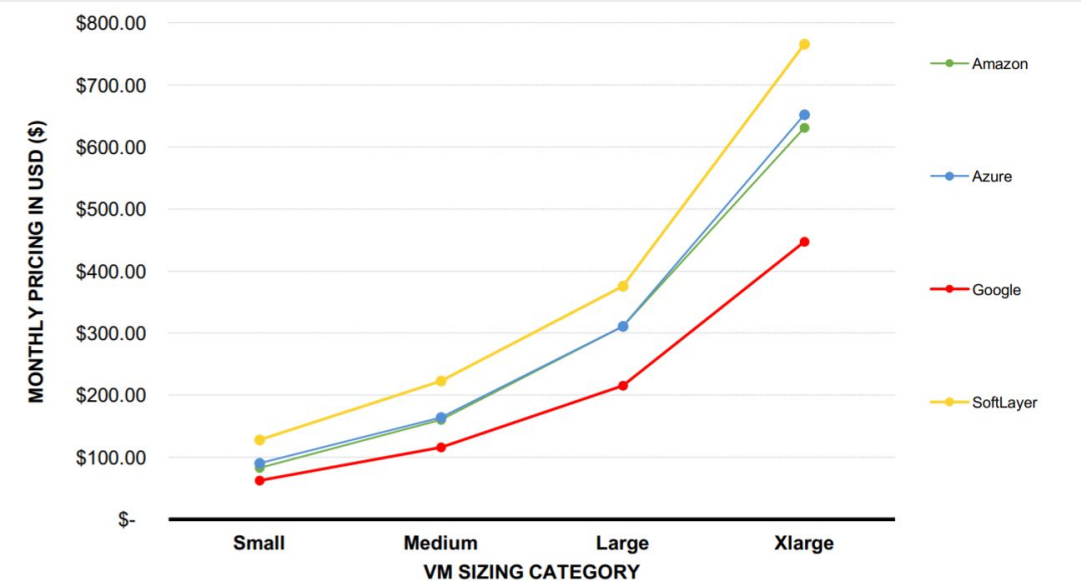


Table 7A: Monthly Cost of VMs Across CSPs

	Small	Medium	Large	Extra Large
Amazon	\$83.00	\$160.27	\$310.54	\$631.08
Azure	\$90.19	\$163.92	\$310.65	\$652.02
Google	\$62.24	\$115.98	\$214.96	\$446.92
SoftLayer	\$128.00	\$223.00	\$376.00	\$766.00

Source: Kinsta

Next Evolution in Cloud Pricing

Google Cloud Subscription Agreement for Public Sector



Provides the “right to use” any GCP product for a period of time for a defined, specified use case [for a fixed price](#)



Provides you with predictability of costs - [no overage fees](#)



Reduce your implementation risk - use [whatever service you need, as much as you need](#), for your project



We’re in this with you! **Google Cloud** has “[skin in the game](#)” with you - [we want your project to be successful](#)



Google Working Toward Optimal HPC Performance

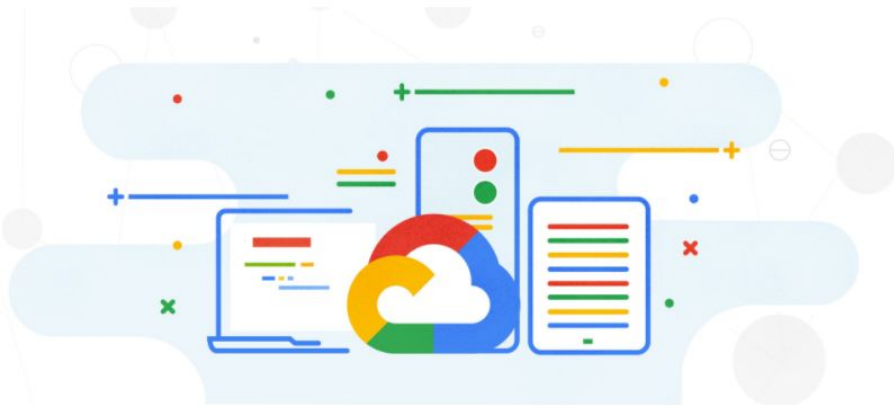


Blog

Menu

HPC

Introducing HPC VM images—pre-tuned for optimal performance



Pavan Kumar
Product Manager

Jason Zhang
Software Engineering Manager

February 2, 2021

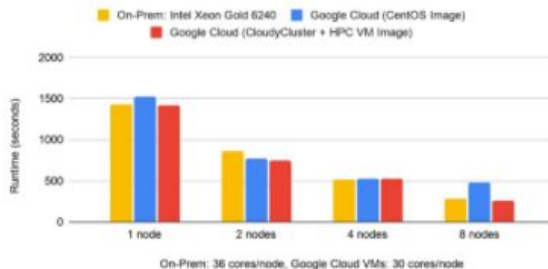
Customer story: Scaling SDPB solver using CloudyCluster and HPC VM image

Walter Landry is a research software engineer in the Caltech [Particle Theory Group](#) working with the international [Bootstrap Collaboration](#). The collaboration uses [SDPB](#), a semidefinite program solver, to study Quantum Field Theories, with application to a wide variety of problems in theoretical physics, such as early universe inflation, superconductors, quantum Hall fluids, and phase transitions.

To expand the collaboration's computation capabilities, Landry wanted to see how SDPB would scale on Google Cloud. Working with [Omnibond CloudyCluster](#) and leveraging the HPC VM image, Landry achieved comparable performance and scaling to an on-premises cluster at Yale, based on Intel Xeon Gold 6240 processors and Infiniband FDR.

Customer Story: Scaling SDPB solver on Google Cloud

Runtime comparison: On-Prem vs. Google Cloud (Lower is better)



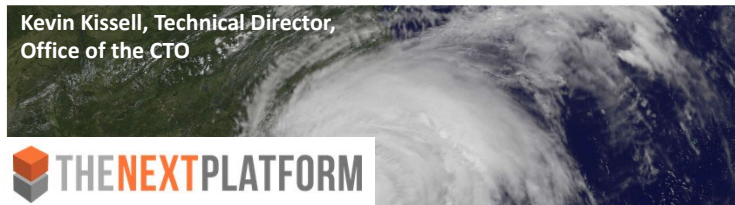
<https://www.googlenewsapp.com/introducing-hpc-vm-images-pre-tuned-for-optimal-performance/>

Google HPC Blog Post

Cloud against the storm: Clemson's 2.1 million VCPU experiment

<https://cloud.google.com/blog/topics/hpc/clemson-experiment-uses-2-1-million-vcpus-on-google-cloud>

Kevin Kissell, Technical Director,
Office of the CTO



THE NEXT PLATFORM

Urgent HPC can Burst Affordably to the Cloud

<https://www.nextplatform.com/2020/01/08/urgent-hpc-can-burst-affordably-to-the-cloud/>



GCP CPU Core Ramp and Count



- 133,573 GCP Instances at peak
- 2,138,000 vCPUs at peak
- 6,022,964 vCPU hours

Processed 2,479,396 hours (~256TB) of video data

- ~4 hours of runtime
- ~1M vCPU within an hour
- ~1.5M vCPU within 1.5 hours
- 2.13M vCPU within 3 hours

Total Cost: \$52,598.64 USD

Average cost of \$0.008 USD per vCPU hour

Architecture - Video



Behind the Scenes of

**cloudycluster**

On

 Google Cloud



DEMO - Video

1. Control Instance Creation
2. Environment Creation



DEMO - Video

3. Job submission through the CCQ Meta-Scheduler to SLURM
4. CCQ instance clean up once the Jobs have completed

CloudyCluster - Architecture - Elastic Slurm Jobs



Questions and Concerns

Next Training Sessions:

- **Data to Dashboard** - [10/21/21]

- **Beginning to End Project Example** - [10/28/21]

Schedule:

<https://jeaimehp.github.io/HackHPC-HPCintheCity21/>

Presenter Contact Information:

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