Breakout Session 3: Track B

Exploration of Cloud-based High Performance Computing

Dr. Albert Lai (Moderator)
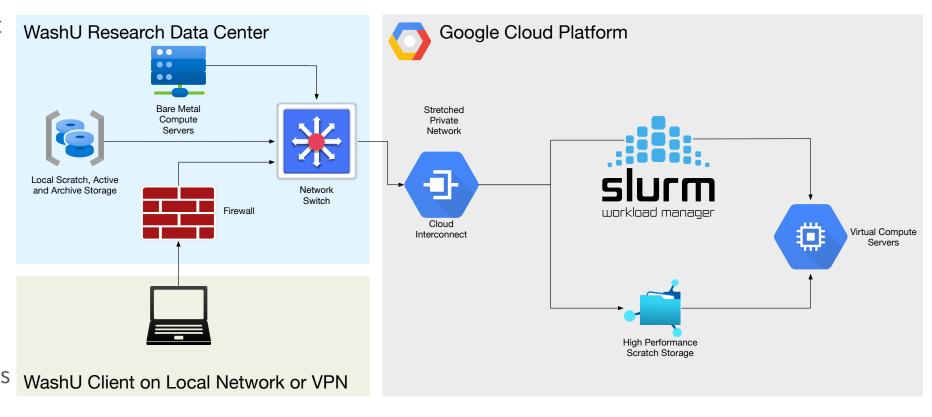*Professor, Washington University in St. Louis*

Specific Aims

- **Aim 1:** Deploy a hybrid-cloud HPC cluster to the public cloud that is seamlessly integrated with on-premises worker nodes and data storage.

- **Aim 2:** Run tests on a range of HPC workloads, including Data Simulations, Bioinformatics, Artificial Intelligence/Machine Learning & Imaging (GPU accelerator-focused), and general interactive workloads. We will compare the performance of workloads running on cloud and on-premises nodes, utilizing job run time and cost as the primary metrics.

- **Aim 3:** Evaluate the viability of deploying HPC clusters and nodes to the public cloud. We will complete this by examining the cost of running the workloads described in Aim 2 and comparing them to the projected costs of traditional on-premises approaches.

Washington University School of Medicine in St. Louis

Hybrid HPC Cluster using GCP Toolkit

- Given the short timeline, needed a fast way to deploy an HPC Cluster in the Cloud.

- GCP Toolkit simplifies the deployment and management of (HPC) clusters on GCP

- Automates cluster setup, configuration, scaling, and monitoring.

- Reduces deployment complexity, accelerates time-to-results, and enhances resource efficiency using the Slurm workload manager

WashU Research Data Center

Bare Metal Compute Servers

Local Scratch, Active and Archive Storage

Firewall

Network Switch

WashU Client on Local Network or VPN

Google Cloud Platform

Stretched Private Network

Cloud Interconnect

slurm
workload manager

Virtual Compute Servers

High Performance Scratch Storage

Washington University School of Medicine in St. Louis

Workloads	Description / Workload type
ArCCH-WGS-VariantCalling	Variant calling pipeline for low Variant Allele Frequency (VAF) Clonal Hematapoiesis
GATK-SV	Structural variation discovery pipeline for WGS
Tensor Machine Learning Model	GPU-focused
Peptide Simulation using CAMPARI	CPU-focused simulation workload
Weather Research & Forecasting Model (WRF)	MPI-type workload
VNC and noVNC Desktops	Interactive workload

Office *of* Health Information *and* Data Science

Washington University School of Medicine in St. Louis

Experiments

Workloads	# Experiments Executed	# Tasks
Dr. Kelly Bolton Lab	13	2,486
Dr. Peter Jin Lab	78	275,572
Dr. Joshua Swamidass Lab	4	63
Dr. Alex Holehouse Lab	4	11,916
Dr. Jian Wang Lab	4	909
Interactive	2	12
Total	105	290,958

Experiments

- 110 Experimental clusters executed
- Permutations of
  - workload type
  - # data sets
  - dynamic/preconfigured server
  - preemptible/persistent configurations

Washington University School of Medicine in St. Louis

Early Observations

- GCP Infrastructure

    - Limit of 7 Slurm clusters per GCP Project (subscription) metadata limitation

    - Regular service disruptions cause job failures every Sunday

    - 70% of Preemptible VMs run less than an hour

    - 14% of Preemptible VMs run for at least 22-24 hours

Early Experimental Results

- 56 Experimental clusters completed successfully
  - Preemptible VMs and infrastructure instability resulted in incomplete experiments
- CPU utilization is higher with VMs configured to match on-premises hosts
- Experiment runtime is less for dynamic CPU resources (VMs sized based on job resource parameters)
- ~50% savings on preemptible VMs
- Compute runtime impacts storage and total costs of experiments
- GCP Filestore (ephemeral scratch storage) cleanup impacts costs of experiments
  - Lack of policy or automation not integrated into workloads replicating on-premise use case

Washington University in St. Louis

SCHOOL OF MEDICINE

Office *of* Health Information
and Data Science

sites.wustl.edu/ohids