Cloud Computing – getting started

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Bioinformatics Workshop
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Why go to the cloud?

- Performance & reliability
- Access to additional storage and compute as needed
- Greater control over compute environment
  - Ability to create persistent web services
- Data sharing needs
- Access to technologies not available on local WashU compute
- It’s a valuable skill? It’s the future?

Why not go to the cloud?

- Cost
- Complexity. Its another thing to learn
- Security?

Public Cloud & in-house compute

- Using the cloud is not the same as using the compute0/1 cluster
  - Not HPC-oriented (no LSF, à la `bsub`; no NFS-based file system)
  - Essence of scientific cloud computing:
    i. Create a VM
    ii. Download Input Data onto VM from Cloud Storage
    iii. Download software onto VM
    iv. Run computation(s)
    v. Upload Output Data on VM to Cloud Storage
    vi. Delete VM

- “research” on the cloud vs. local in-house compute
  - Exploratory compute on the cloud can get expensive very quick.
  - Try to do small-scale “research” on in-house compute, and then move to the cloud for large-scale “production” tasks
  - Use the cloud for functionality not supported by local compute
  - Use the cloud as a backup when local system is unstable

Getting started - Overview of intial steps

1. **Initial setup**. Request an AWS or GCP cloud account from WUIT
2. **POs**. Request a purchase order from your department and link to the account and encumber with appropriate sources of funding
3. **Login**. Test login and user permissions to access billing information and other necessary functionality. Request additional permissions from WUIT as needed.
4. **Users**. Request addition of users from the lab who need access
5. **Invoices**. Set up routing of DLT (AWS) or Burwood (GCP) bills to your email
6. **Alerts**. Set up billing dashboards and monthly billing alerts.
7. **Cost control**. Consider cost optimizations such as reserved instances

Initial setup with WASHU IT

- WASHU IT Cloud Computing Service
  - https://it.wustl.edu/services/cloud-computing/
- Benefits of using WASHU IT
  - University negotiated, policy compliant contracts with select public cloud vendors
  - Account Management
  - University Billing
  - Access to cloud consoles via WUSTL Key login
  - HIPAA BAA (select vendors)
  - Service Discounts
- Public Cloud Providers
  - https://it.wustl.edu/services/cloud-computing/cloud-computing-services-comparison/
  - Google Cloud Platform (GCP)
    i. https://it.wustl.edu/services/cloud-computing/google-cloud-platform/
  - Amazon Web Services (AWS)
    i. https://it.wustl.edu/services/cloud-computing/amazon-web-services/
  - Microsoft Azure
    i. https://it.wustl.edu/services/cloud-computing/microsoft-azure/
- Contacts
  - John Bailey (jwbailey@wustl.edu) and Steven Clement (csteven@wustl.edu)
  - Please submit all initial requests for cloud accounts through the above web forms

Project initiation – request a new GCP “project” or AWS “account”

Washington University in St. Louis

Information Technology

SERVICES I WANT TO HELP IT STRATEGIC PLAN MORE

Google Cloud

Google Cloud

Google Cloud (formerly GCP) is a newer public cloud platform geared toward research computing and storage. For information on Google Cloud, reference the following Google web pages:

- Google Cloud Service Catalog
- Google Cloud Pricing Calculator
- Google Cloud Service Status
- Google Cloud Technical Documentation

Ready to get started with Google Cloud?

1. Review the Cloud Computing: Features & Options service description to understand what is included and excluded
2. Request a new WashU Google Cloud project

Already have a WashU GCP project?

- Login to the Google Cloud console using your WUSTL Key
- Contact us to request access to an existing WashU Google Cloud project

Washington University in St. Louis

Information Technology

SERVICES I WANT TO HELP IT STRATEGIC PLAN MORE

Amazon Web Services

amazon web services

Amazon Web Services (AWS) is the industry leader in public cloud. AWS provides a range of services including compute, storage, and databases. For information on AWS, reference the following Amazon web pages:

- AWS Service Catalog
- AWS Product Availability by Region
- AWS Pricing Calculator
- AWS Service Status
- AWS Technical Documentation
- AWS Service Limits

Ready to get started with AWS?

1. Review the Cloud Computing: Features & Options to understand what is included and excluded
2. Request a new WashU AWS account

Already have a WashU AWS account?

- Login to the AWS Portal using your WUSTL Key
- Contact us to request access to an existing WashU Azure subscription

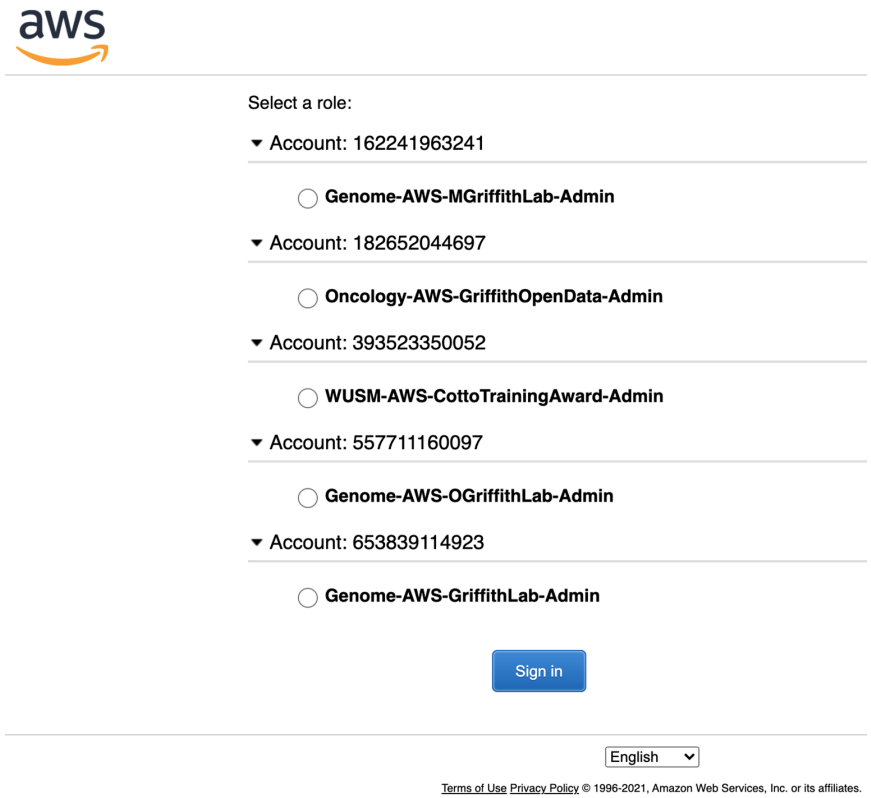
Billing, POs, encumbering ...

- Billing contacts within each department open a standing/blanket Purchase Order (POs) with each provider or reseller
  - Billing contacts vary by Department:
- You may establish multiple WASHU POs and link these to particular cloud accounts or you can just use one for Google/Burwood or AWS/DLT
- You will be asked periodically to encumber the PO for a certain amount based on how much you project to spend over the next 6-12 months
  - At this point you decide how much will be sourced to which fund numbers

Relationship with WASHU Resellers

- For billing and legal purposes WASHU has established business agreements with resellers
  - DLT (AWS)
  - Burwood Group (GCP)
- Interaction with these resellers can be quite limited
  - Does add some complexity to billing because what you see in the cloud billing console is not necessarily what you will be charged by DLT or Burwood (may be less or more)

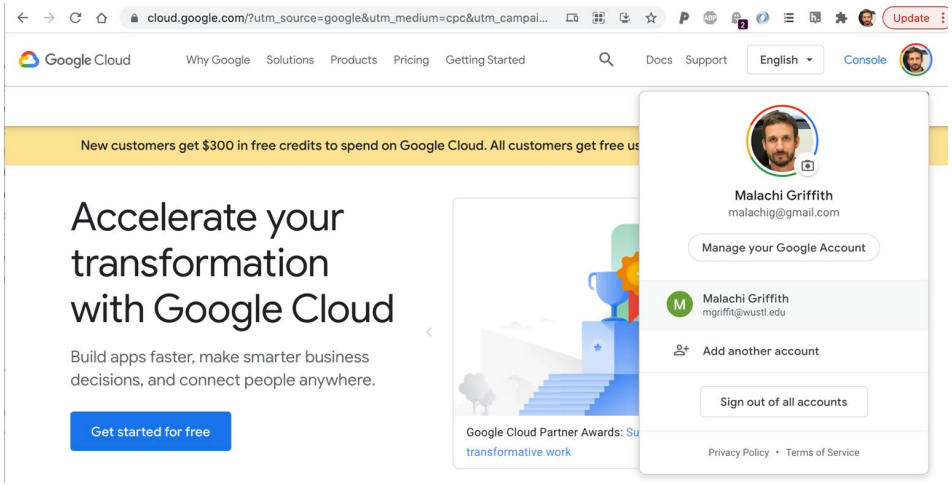
Logging in to AWS (http://connect.wustl.edu/awsconsole)

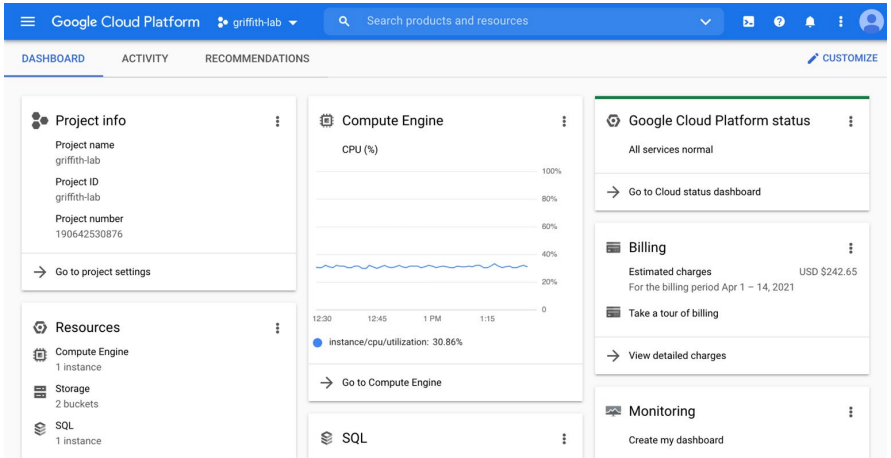


- Authentication uses your WUSTL Key
- You can have multiple accounts (optional)
  - Per project
  - Per billing source
- Or you have can one account and manage billing by paying one bill from multiple sources
- Multiple accounts can also be used to compartmentalize access to members of the lab working on different projects
- Each account will generate distinct billing, billing alerts, etc.

Logging into GCP (https://cloud.google.com/)

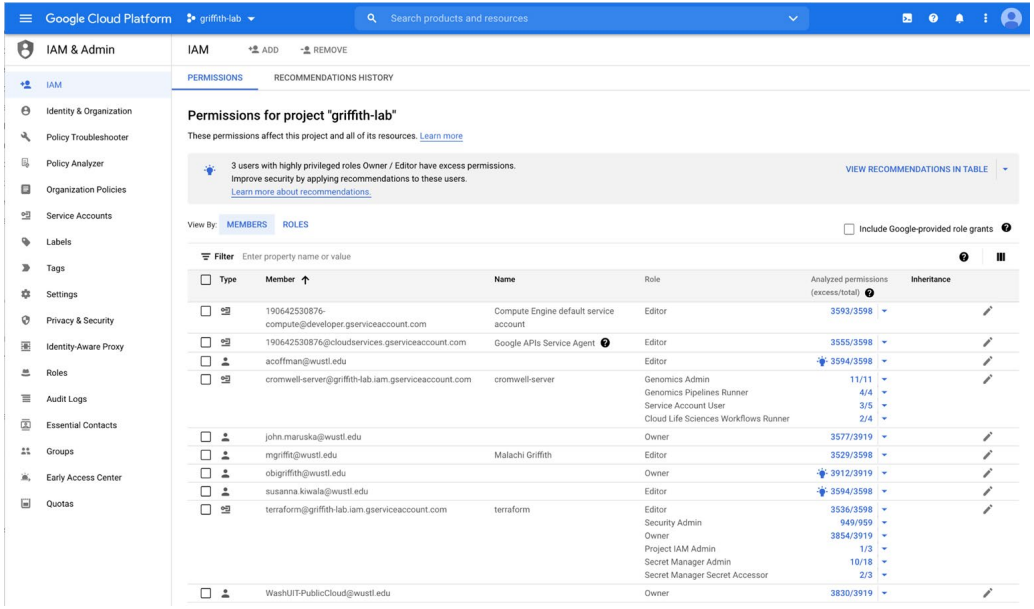
- Request a WASHU Google account
  - A very limited functionality Google account associated with your WASHU login
  - You now have two Google accounts. If you use the Google ecosystem a lot, this will be annoying.
  - Better functionality would happen with Google Workspace (formerly known as “G Suite”) integration; however, WashU IT is very invested with Microsoft and isn’t motivated yet to do this.





Adding users from a lab to a cloud account

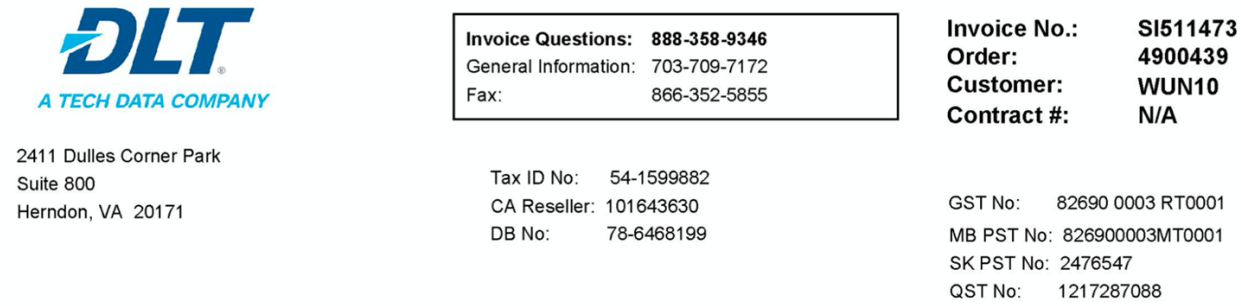
- For AWS, the ability to add users from the lab to access AWS accounts is managed through WUIT by email
  - No way for PI to see what users are currently authorized without asking WUIT
- For GCP, the ability to add users is also limited to WUIT but at least it is possible to view the current configuration
  - You can get permission to add users yourself



Funding Opportunities

- NIH STRIDES Partnership
  - https://cloud.cit.nih.gov/
- AnVIL Cloud Credits (AC2) Program
  - https://anvilproject.org/news/2021/04/12/announcing-anvil-cloud-cost-credits-program
- AWS Programs for Research and Education
  - https://aws.amazon.com/grants/
- GCP Education Credits
  - https://cloud.google.com/billing/docs/how-to/edu-grants

AWS/DLT Invoice example



DLT
A TECH DATA COMPANY

2411 Dulles Corner Park
Suite 800
Herndon, VA 20171

Invoice Questions: **888-358-9346**
General Information: 703-709-7172
Fax: 866-352-5855

Tax ID No: 54-1599882
CA Reseller: 101643630
DB No: 78-6468199

Invoice No.: **SI511473**
Order: **4900439**
Customer: **WUN10**
Contract #: **N/A**

GST No: 82690 0003 RT0001
MB PST No: 826900003MT0001
SK PST No: 2476547
QST No: 1217287088

Bill To: Washington University in St. Louis
Accounts Payable
Campus Box 1056
700 Rosedale Ave
SAINT LOUIS, MO 63112-1408

Ship To: Washington University in St. Louis
Accounts Payable
ONCOLOGY / SCB
425 SOUTH EUCLID
SOUTHWEST TOWER
SAINT LOUIS, MO 63108

Date	Period of Performance	ACT # / PDN #		Terms		
02/26/21	01/01/21 - 01/31/21			Net 30 Days		
Purchase Order Number		**Order Date**	**Salesperson**	**Our Order Number**		
2940074K		02/26/21	Jennifer Triplett	4900439		
Quantity		**CLIN No.**	**Item Number**	**Tax**	**Unit Price**	**Amount**
Req.	**Ship**	**B.O.**	**Description**			
1	1		6538-3911-4923 **413500**	N	1,491.27	1,491.27

AWS 01-2021 - WUSTL McDonnell Genome Institute

Invoices will be emailed to you monthly for approval. Work with DLT to ensure the right people get emailed.

- Performance Period
- WASHU PO
- AWS Account #

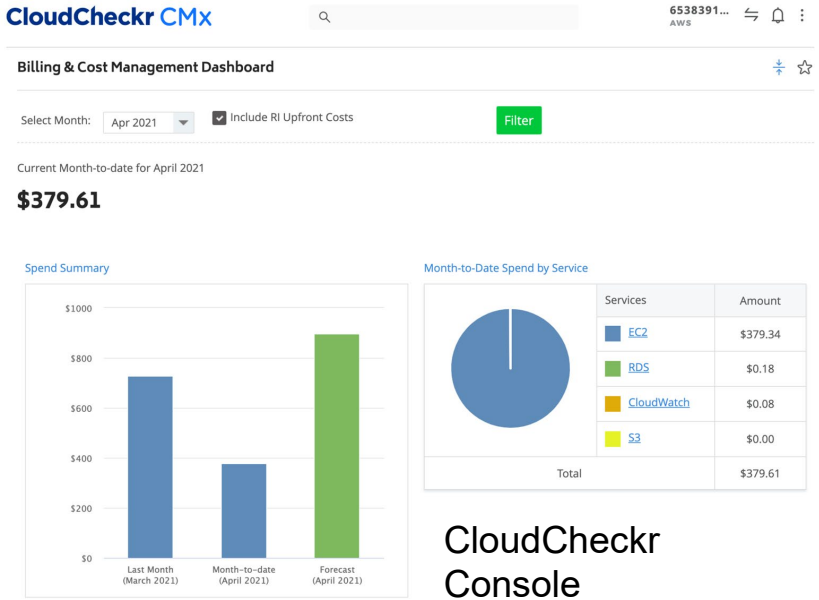
AWS/DLT Invoice example

Description	Qty	Rate	Price
4900439 - 6538-3911-4923 - McDonnell Genome Institute - Genome Griffith Lab			
CloudWatch			
Alarm metric month (standard resolution) - US West (Oregon)	2	0.09500	0.19
GB-mo of log storage - US East (Northern Virginia)	0.01	0.00000	-
GB-mo of log storage - US West (Oregon)	0	0.00000	-
CloudWatch Total	**2.01**	**0.03167**	**0.19**
DynamoDB			
GB - first 10 TB / month data transfer out beyond the global free tier	0	0.00000	-
GB - next 40 TB / month data transfer out	0	0.00000	-
DynamoDB Total	**0**	**0.00000**	**-**
EC2			
Elastic IP address not attached to a running instance per hour (prorated)	2231	0.00475	10.60
EUN1-AWS-Out-Bytes in EU (Stockholm)	0	0.00000	-
GB - first 10 TB / month data transfer out beyond the global free tier	1738.81	0.08550	148.67
GB - regional data transfer - in/out/between EC2 AZs or using elastic IPs or ELB	26.48	0.00944	0.25
GB - US West (Oregon) data transfer to Asia Pacific (Mumbai)	0	0.00000	-
GB - US West (Oregon) data transfer to Asia Pacific (Seoul)	0.01	0.00000	-
GB - US West (Oregon) data transfer to Asia Pacific (Singapore)	0.23	0.00000	-
GB - US West (Oregon) data transfer to Asia Pacific (Sydney)	0	0.00000	-
GB - US West (Oregon) data transfer to Asia Pacific (Tokyo)	0.06	0.00000	-
GB - US West (Oregon) data transfer to AWS GovCloud (US)	0.02	0.00000	-
GB - US West (Oregon) data transfer to Canada (Central)	0.23	0.00000	-
GB - US West (Oregon) data transfer to EU (Germany)	0.01	0.00000	-
GB - US West (Oregon) data transfer to EU (Ireland)	1.3	0.01538	0.02
GB - US West (Oregon) data transfer to EU (London)	0	0.00000	-
GB - US West (Oregon) data transfer to EU (Paris)	0	0.00000	-
GB - US West (Oregon) data transfer to South America (Sao Paulo)	0	0.00000	-
GB - US West (Oregon) data transfer to US East (Northern Virginia)	19.4	0.01907	0.37
GB - US West (Oregon) data transfer to US East (Ohio)	0.27	0.03704	0.01
GB - US West (Oregon) data transfer to US West (Northern California)	0	0.00000	-
GB-month of General Purpose SSD (gp2) provisioned storage - US West (Oregon)	2560	0.09500	243.20
GB-Month of snapshot data stored - US West (Oregon)	1824.65	0.04750	86.67
In Asia Pacific (Hong Kong)	0.02	0.00000	-
In Middle East (Bahrain)	0	0.00000	-
On Demand Linux m5.2xlarge Instance Hour	744	0.36480	271.41
On Demand Linux m5a.2xlarge Instance Hour	744	0.32680	243.14
On Demand Linux t2.large Instance Hour	744	0.08816	65.59
On Demand Linux t2.medium Instance Hour	744	0.04409	32.80

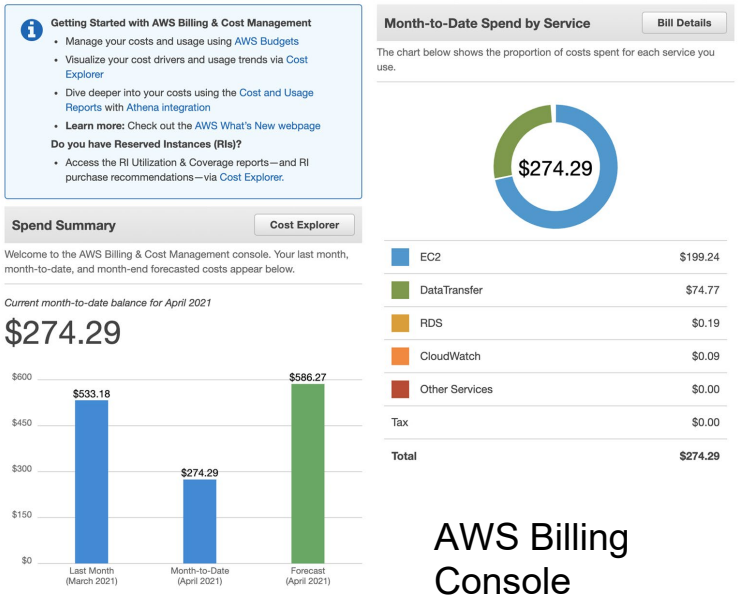
- DLT gives a detailed breakdown of cloud services you are being charged for
- This only loosely corresponds to the billing information you see in AWS console
  - The usage should be the same, but *how* you are billed for it can be very different
  - We have seen DLT bills >2x what is shown in AWS
  - Related to reserved instances. DLT calls this “RI arbitrage”. Basically DLT is reserving instances, keeping the savings from Amazon and billing you the full agreed rate.

CloudCheckr CMx (https://app-us.cloudcheckr.com/)

- More detailed information on what DLT will actually charge you for AWS usage
- Must request that DLT set this up for you



CloudCheckr Console



AWS Billing Console

Google / Burwood Invoice example

Invoices will be emailed to you monthly for approval. Work with Burwood to ensure the right people get emailed.

- Performance Period
- WASHU PO
- Google Project

INVOICE - 02_23_WASUNI-Oncology - Griffith

Billing Interval: 02-01-23 - 02-28-23

Invoice Date: 02-28-23

Purchase Order: PO00021529

burwood group, inc.

CUSTOMER

Washington University in St. Louis

Group: Oncology - Griffith
7425 Forsyth Blvd
Clayton, 63105

CONTACT

Burwood Group Inc

8582 Solutions Center
Chicago, IL 60677, United States

CLOUD PROJECT SUMMARY

Griffith-Lab (Purchase Order: PO00021529): $365.30
Terra-5f2dd205 (Purchase Order: PO00021529): $0.16
Terra-D3606022 (Purchase Order: PO00021529): $0.16

Terra-1a888a14 (Purchase Order: PO00021529
Terra-8eb53bf4 (Purchase Order: PO00021529

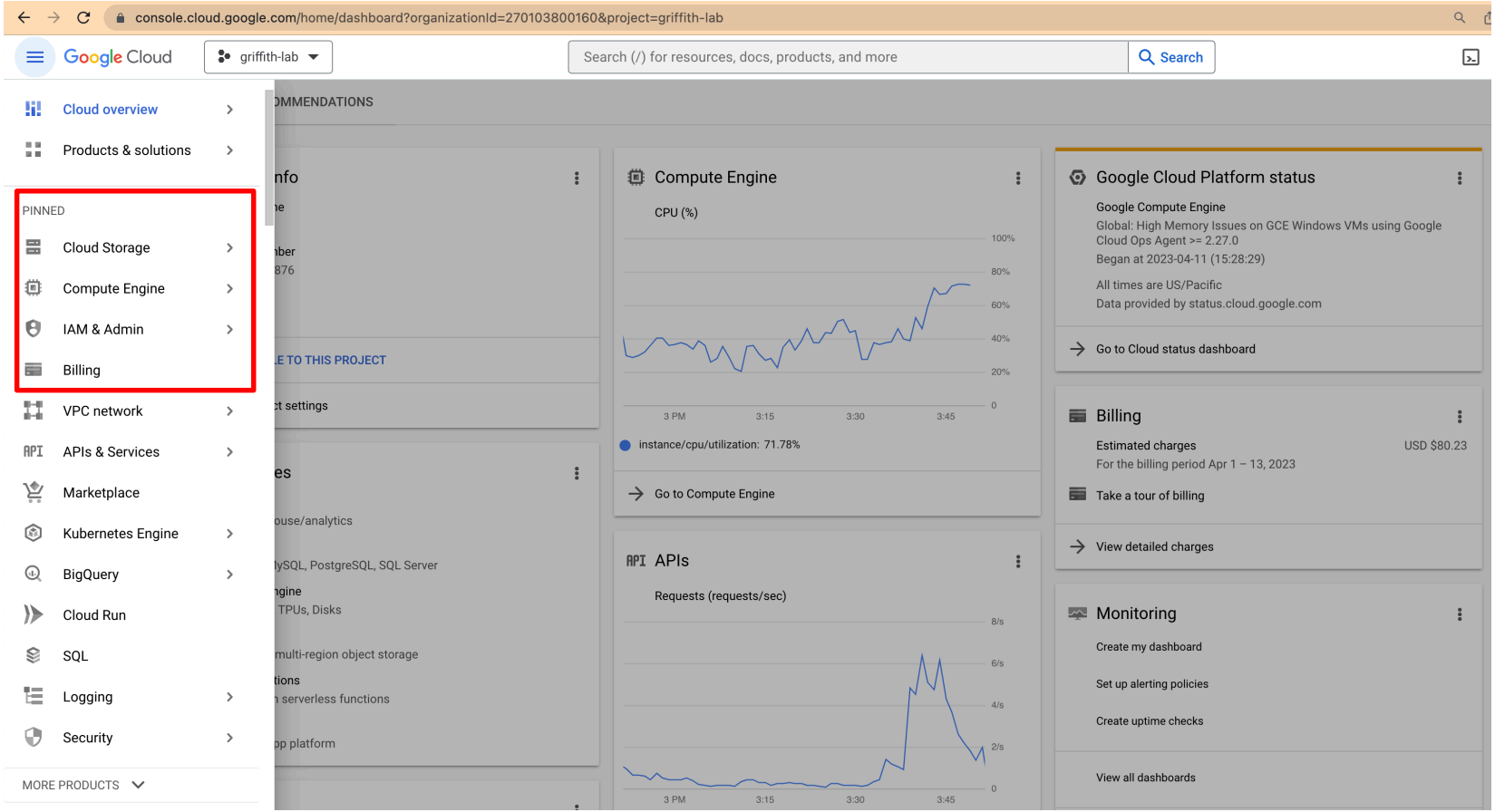
Total: $365.94

DETAILS

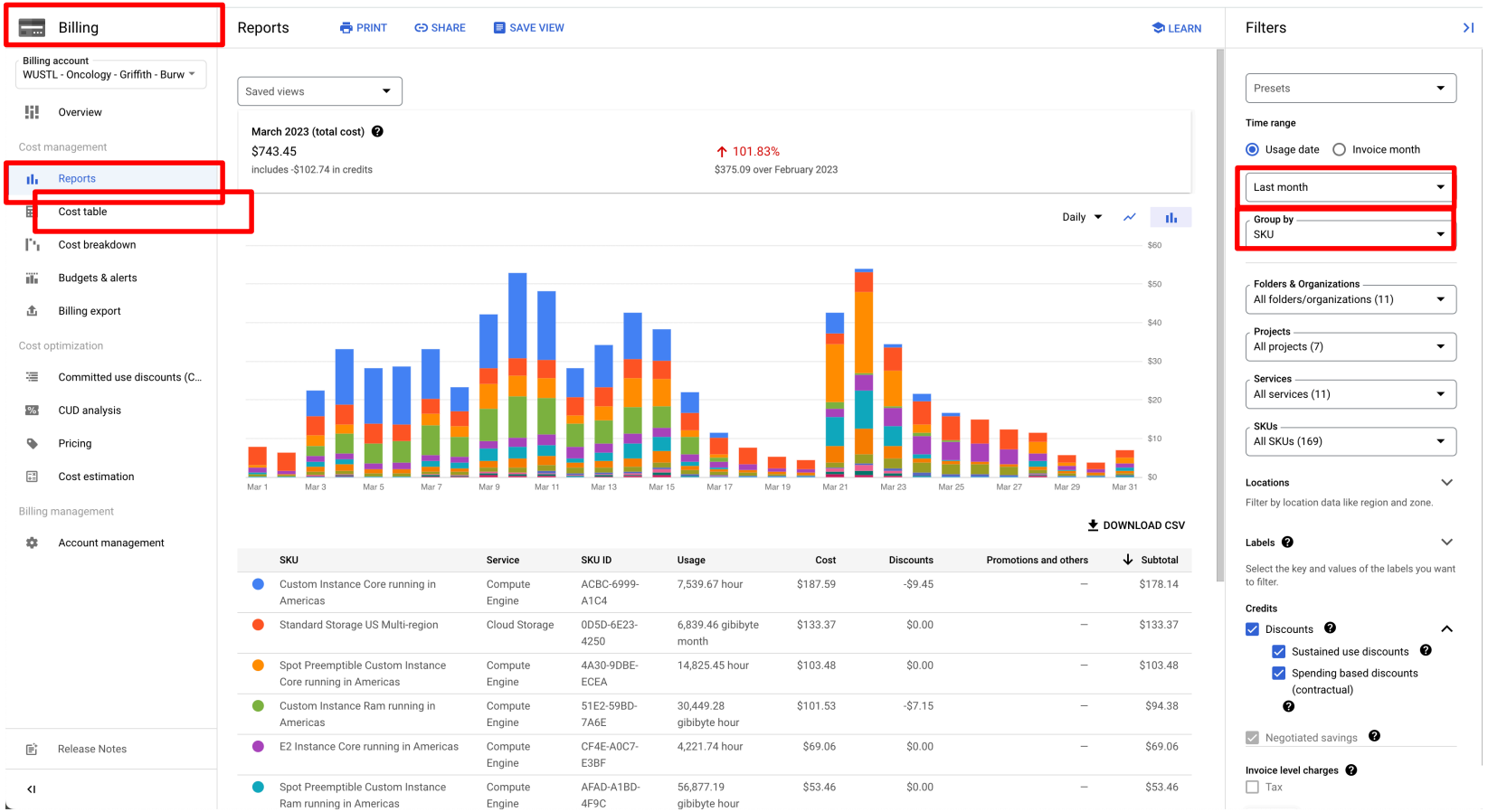
Griffith-Lab (Purchase Order: PO00021529)

SERVICE	LIST PRICE	I2 DISCOUNT	PROMOTIONS	ADJUSTMENTS	TOTAL
Cloud Storage	$166.47	$-7.93	$-34.34	$0	$124.20
Compute Engine	$254.56	$-12.12	$-1.35	$0	$241.10
TOTAL	$421.04	$-20.05	$-35.69	$0	$365.30

The google cloud console - https://console.cloud.google.com/

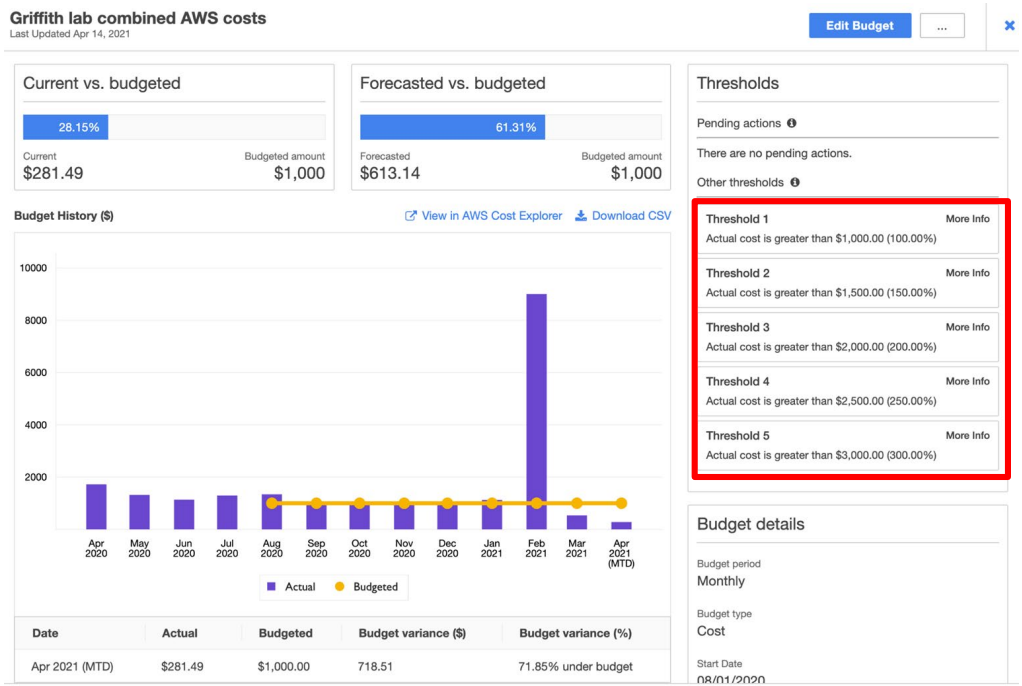


Google Billing Dashboard



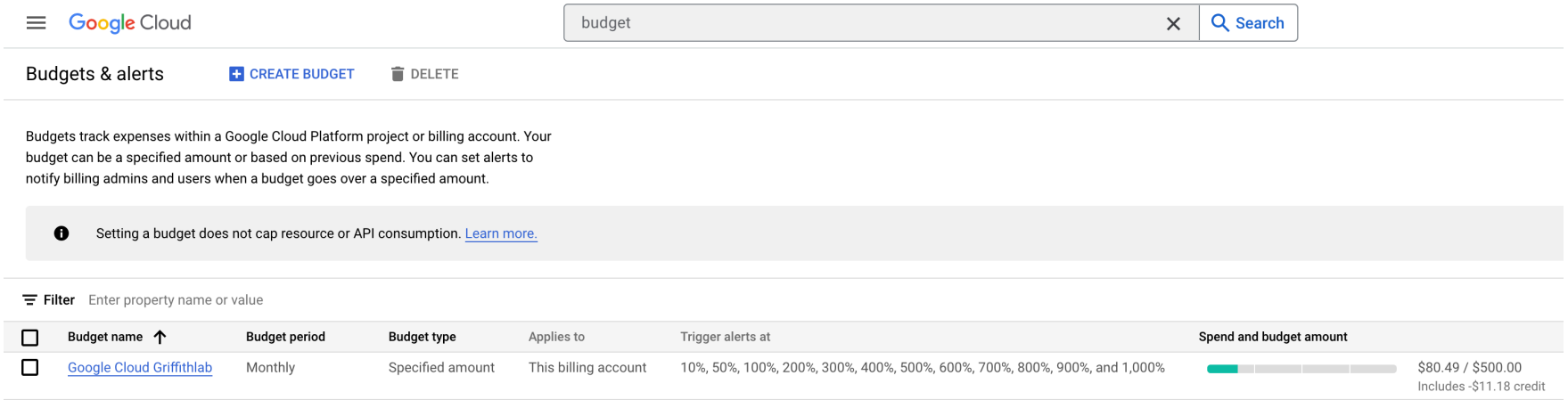
“Budgets” and Billing Alerts in AWS

- Creating a “budget” in AWS allows you to set up email/text alerts when you hit certain amounts each month
- Do this!



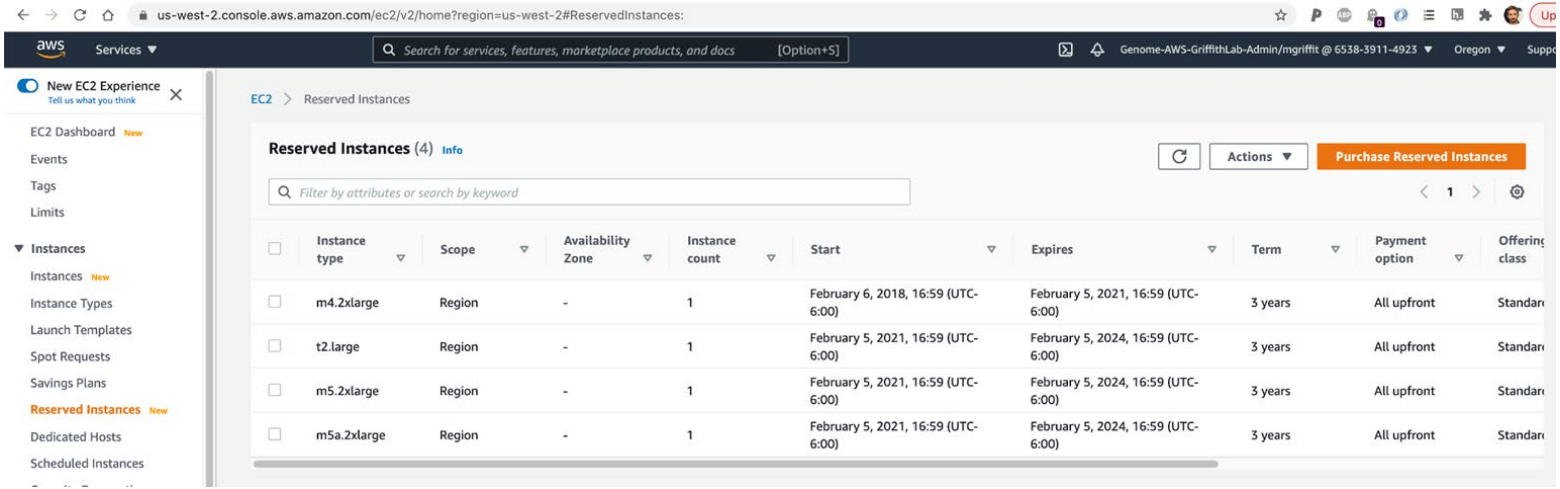
“Budgets” and Billing Alerts in GCP

- Creating a “budget” in GCP allows you to set up email/text alerts when you hit certain amounts each month
- Do this!



Long-Term Compute:
“Reserved Instances” (AWS) and “Commitments” (GCP)

- If you have persistent compute services running use of Reserved Instances or Commitments can result in huge savings
  - E.g. by reserving instances for 3 years at a cost of ~$8,000 we project savings of ~$15,000 compared to if we just used on demand resources for that whole time



Short-Term Compute:
“Spot” (AWS) or “Preemptible” (GCP) Instances

- Meant for “short-term” fault-tolerant jobs
- Much cheaper pricing (up to 90% at times) than regular compute instances
- Drawback is that AWS or GCP reserves the right to take back the machine at any given time depending on the state of the cloud
- Google Preemptible Instances can run at most for 24 hours
- See GCP Preemptible VM Instances or Amazon EC2 Spot for more details
- Often useful for running many batch jobs at scale cheaply

Introduction to general AWS cloud computing concepts

Introduction to AWS

« Prerequisites Course Log into AWS »

Preamble

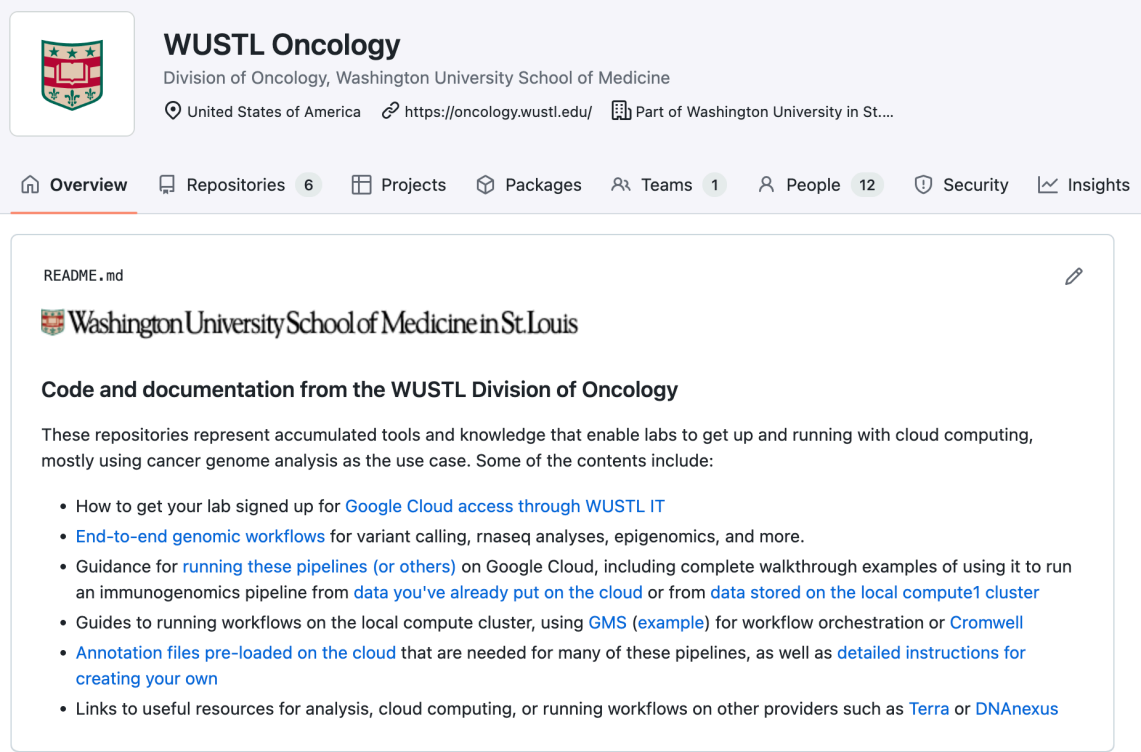
Cloud computing allows users to quickly access an arbitrary amount of compute resources from a distance without the need to buy or maintain hardware themselves. There are many cloud computing services. This tutorial describes the use of the Amazon Web Services (AWS) elastic compute (EC2) resource. However, the fundamental concepts covered here will generally apply to other cloud computing services such as Google Cloud, Digital Ocean, Microsoft Azure, etc., though with substantial differences in jargon used by each provider.

Table of Contents

1. Acknowledgements
2. Glossary and abbreviations
3. What do I need to perform this tutorial
3. What do I need to perform this tutorial
   3.1 Creating an account
   3.2 Logging into the AWS console
4. What is a Region?
5. How much does it cost to use AWS EC2 resources?
   5.1 How does billing work?
6. Necessary steps for launching an instance
   6.1 Step 1. Choosing an AMI
   6.2 Step 2. Choosing an instance type
   6.3 Step 3. Configuring instance details
   6.4 Step 4. Adding storage
      6.4.1 Storage volume options
   6.5 Step 5. Tagging the instance
   6.6 Step 6. Configuring a security group
   6.7 Step 7. Reviewing the instance before launch
   6.8 Step 8. Assigning a key pair
   6.9 Step 9. Reviewing launch status
   6.10 Step 10. Examining a new instance in the ec2 console
   6.11 Step 11. Logging into an instance
7. Trouble-shooting and advanced topics
   7.1 Can not login to EC2 instance - what might have gone wrong?
   7.2 How do storage volumes appear within a linux instance on amazon EC2?
   7.3 Taking stock of compute resources within an ubuntu linux instance
   7.4 Basic setup and administration of an ubuntu linux instance
   7.5 Setting up an Apache web server
   7.6 What is difference between the start, stop, reboot and terminate instance states?
   7.7 How do I create my own AMI, publish as a Community AMI, and what is a snapshot?

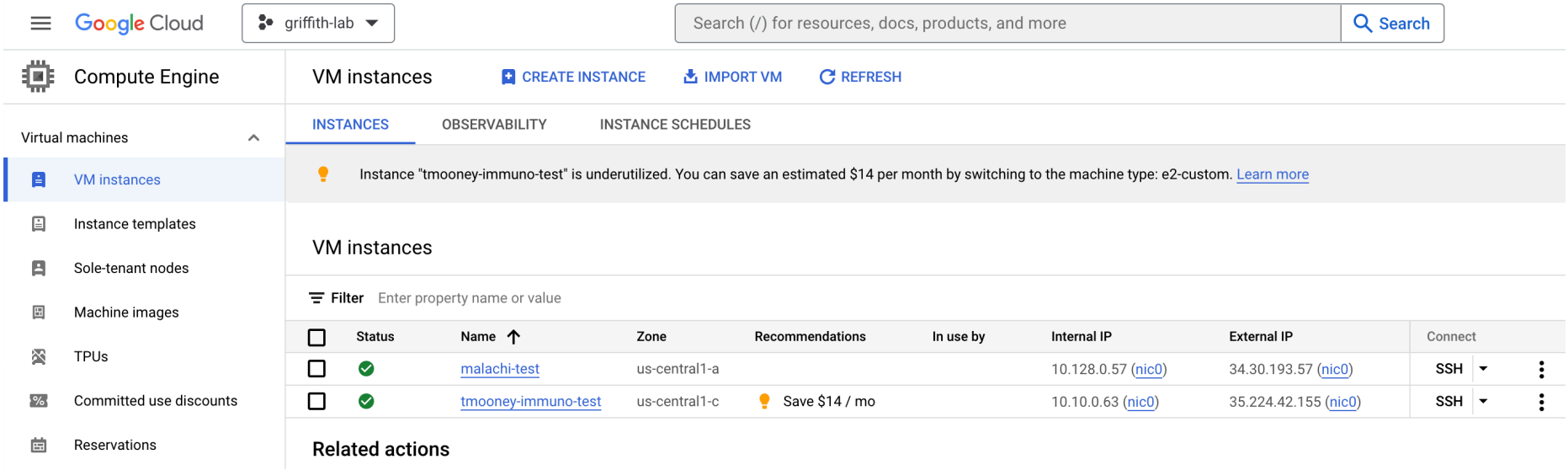
https://rnabio.org/module-00-setup/0000/06/01/Intro_to_AWS/

Okay, I’m ready to actually do something on the cloud…



https://github.com/wustl-oncology

Launch an instance from the console and login



https://console.cloud.google.com/

The Google Cloud SDK – working with data in buckets

https://cloud.google.com/sdk/docs/install (OR https://hub.docker.com/r/google/cloud-sdk/)

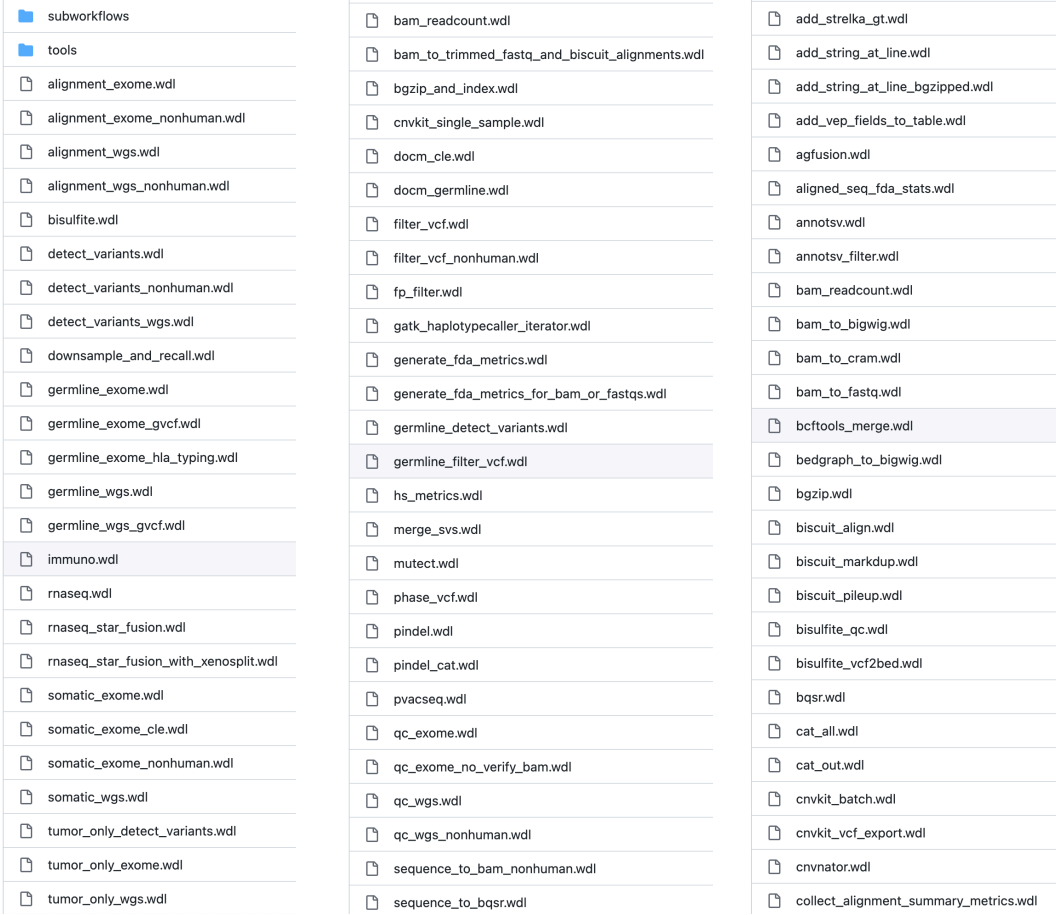
- gcloud auth login
- gcloud config list
- gsutil ls
- gsutil cp

```
mgriffit@3071-AL-05015 ~ % gsutil ls
gs://griffith-lab-malachi-adhoc/
gs://griffith-lab-test-kartik/
gs://griffith-lab-test-layth/
gs://griffith-lab-test-malachi/
gs://griffith-lab-test-tmooney/
gs://griffith-lab-workflow-inputs/
gs://griffith-lab-zls_dev-immuno-pipeline/
mgriffit@3071-AL-05015 ~ %
```

Perform an ad hoc analysis in a single Google VM

https://github.com/wustl-oncology/immuno_gcp_wdl_compute1/blob/main/AdHoc.md

Running WDL pipelines on the Google Cloud



Running a WDL pipeline on Google, in simple terms involves:

- Identifying the specific WDL pipeline you wish to use
- Create a YAML file that describes the inputs/parameters needed for that pipeline (including your data)
- Upload input data to a Google bucket
- Start a Google Virtual Machine (VM) running Cromwell and log into it
- Use Cromwell to run the WDL pipeline with your YAML inputs

- Cromwell manages all resources on Google Cloud
- Once complete results can be stored in a cloud bucket or downloaded locally
- We have created tools (python) to facilitate the above step

https://github.com/wustl-oncology/analysis-wdls

An end-to-end tutorial that runs immuno.wdl on public data

Running the WASHU Immunogenomics Workflow on Google Cloud - compute1 version

Preamble

This tutorial demonstrates how to run the WASHU immunogenomics pipeline (immuno.wdl) on Google Cloud. This will be done by first setting up the workflow definitions, input data and reference files and a YAML config file on a user's local system. The user will also set up a Google Cloud environment and all the inputs will be staged to this cloud environment. Next Cromwell will be used to execute the pipeline using the specified input and reference files, and finally the results will be pulled back to the local system and cloud resources will be cleaned up.

This version assumes that your are staging your input data files from the WASHU RIS storage1/compute1 cluster. Some steps are run within docker containers on that cluster. It therefore requires that you have access to storage1 disk and ability to launch jobs on compute1 using LSF (bsub).

Source of instructions

This tutorial is a specific example of how to run a specific pipeline (immuno) on a specific example dataset (HCC1395 Tumor/normal cell line pair). The steps below are taken from the following link where you will find a more generic set of documentation that explains in detail how to run any WDL pipeline on the Google Cloud using tools created to assist this process. https://github.com/wustl-oncology/cloud-workflows/tree/main/manual-workflows

Prerequisites

- google-cloud-sdk
- git

Security

https://github.com/wustl-oncology/immuno_gcp_wdl_compute1