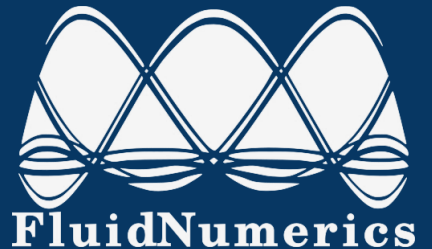


Fluid Numerics

Research Computing Cloud
XSEDE



About us

- Started Community Development & Outreach in 2017 in Boulder, CO
- “Service for Science” Mission
 - 2018 gpuhackathon.com > oshackathon.org
 - 2020 WATERCHaNGE NPO
- Actively involved in government funded research
 - Topographic Dynamics of the Gulf Stream (FSU)
 - Fast Equilibration of Ocean Tracers Software (FEOTS; LANL)
- Actively involved in open-source projects
 - TrixiFramework/HOHQMesh
 - RocmSoftwarePlatform/HIPFort
 - SchedMD/slurm-gcp

Our vision

Broad view

- Bridge gaps between commercial technology vendors and academic research
- Provide Research Computing as a Service (RCaaS)
- Contribute to open-source projects that enable research

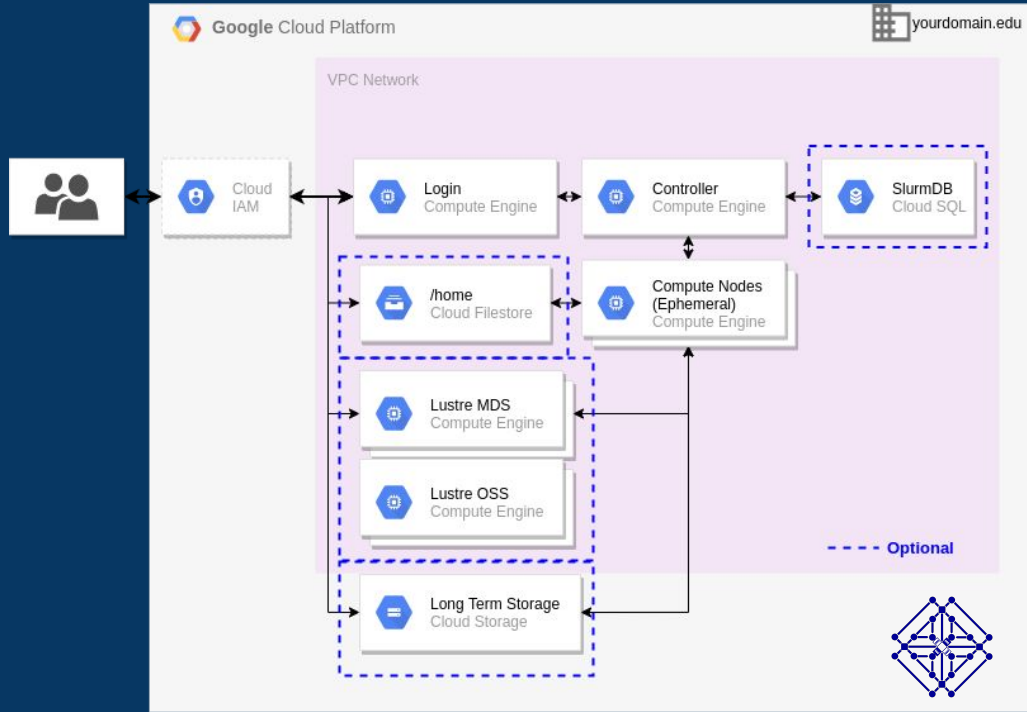
Solutions

- Research Computing Cloud
 - Open Source Solutions
 - WATERCHaNGE OCEAN Cluster
- Portable GPU Programming Training
 - ROCm Lunch & Learns
 - 3-day Virtual Hands-on Training
 - 5-day Mentored Sprints

Publicly Available Codelabs

<https://github.com/FluidNumerics/scientific-computing-edu>

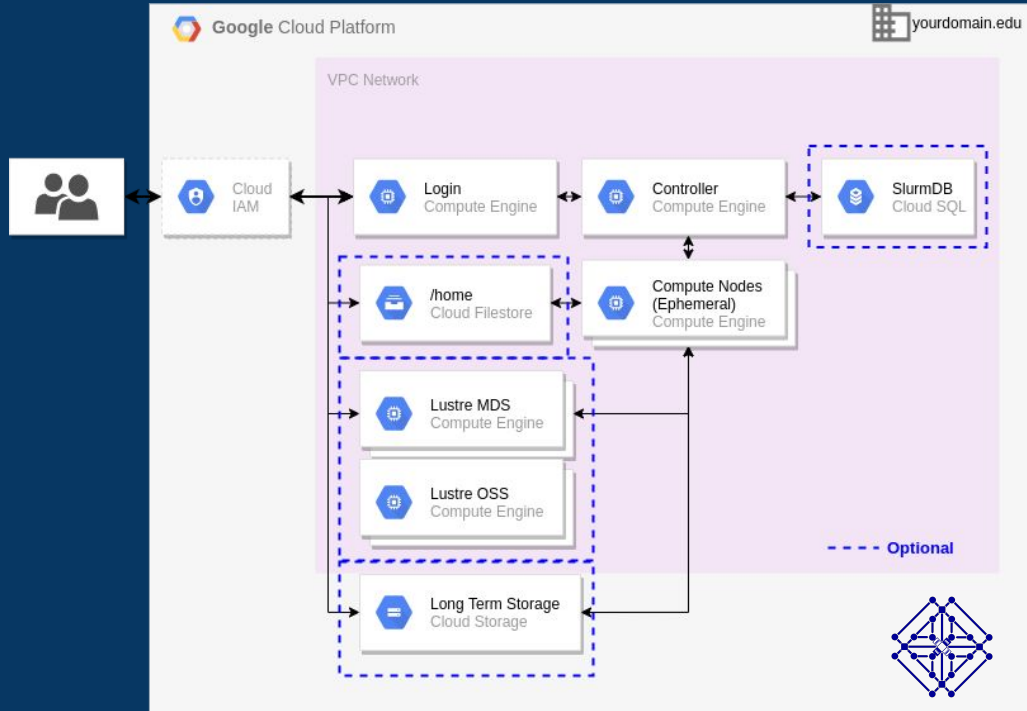
Research Computing Cloud



Replicate on-premise look & feel

- Slurm Workload Manager
- Login Node(s) with SSH access
- NFS Storage Integrations
- Lustre Storage Integrations
- Environment/Spack Modules
 - Multiple Compilers and MPI Builds
 - Singularity Containers
 - Commonly used Software in Research Computing

Research Computing Cloud



Expose Cloud Benefits

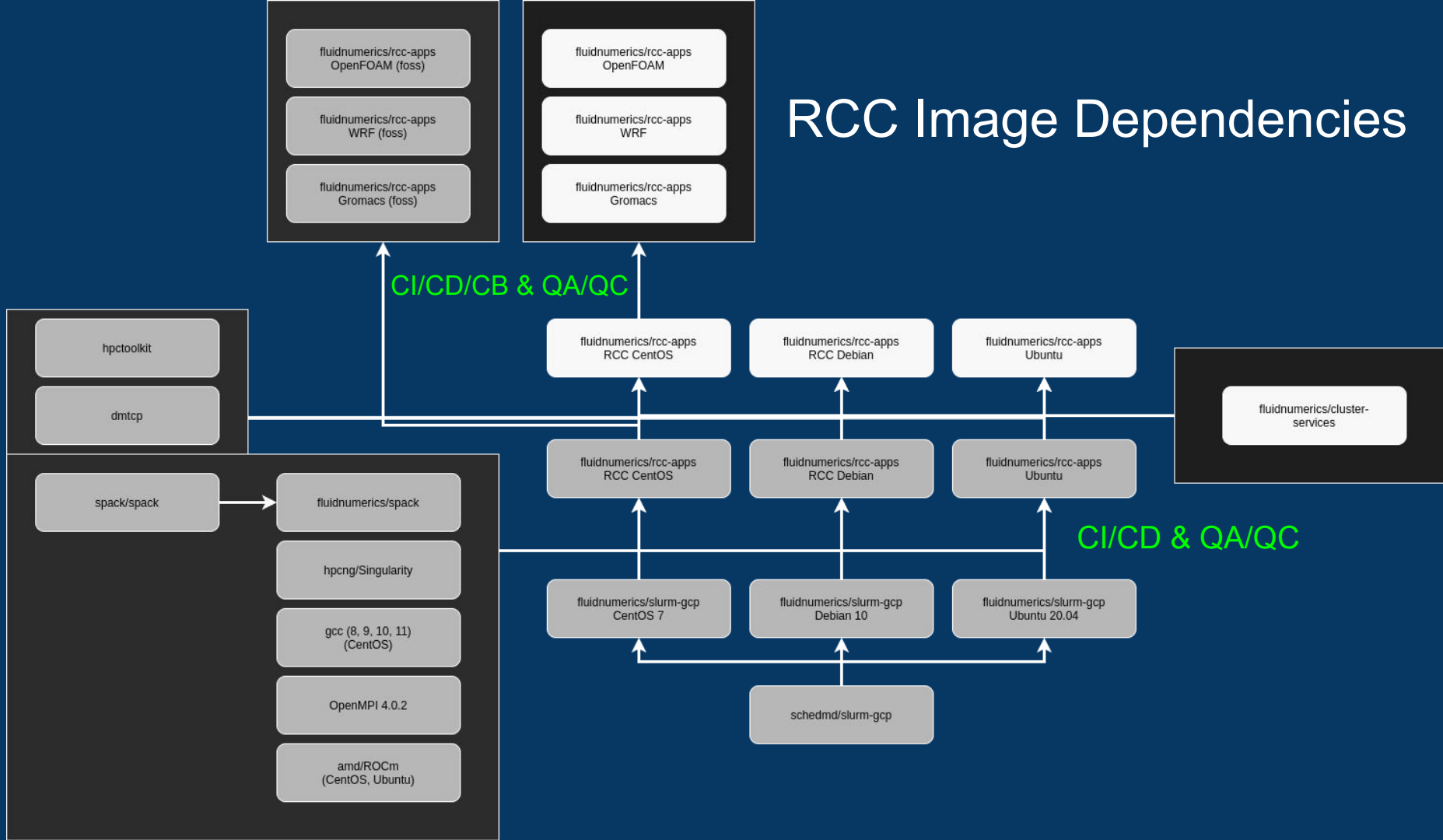
- Ephemeral Auto-Scaling compute nodes
- Multi-partition for heterogeneous compute resources
- Multi-zonal (High Availability)
- Multi-regional (Globally Scalable)
- Multi-Project (Granular Billing)
- Deploy applications
 - Singularity containers
 - VM images
 - Traditional builds

Research Computing Cloud

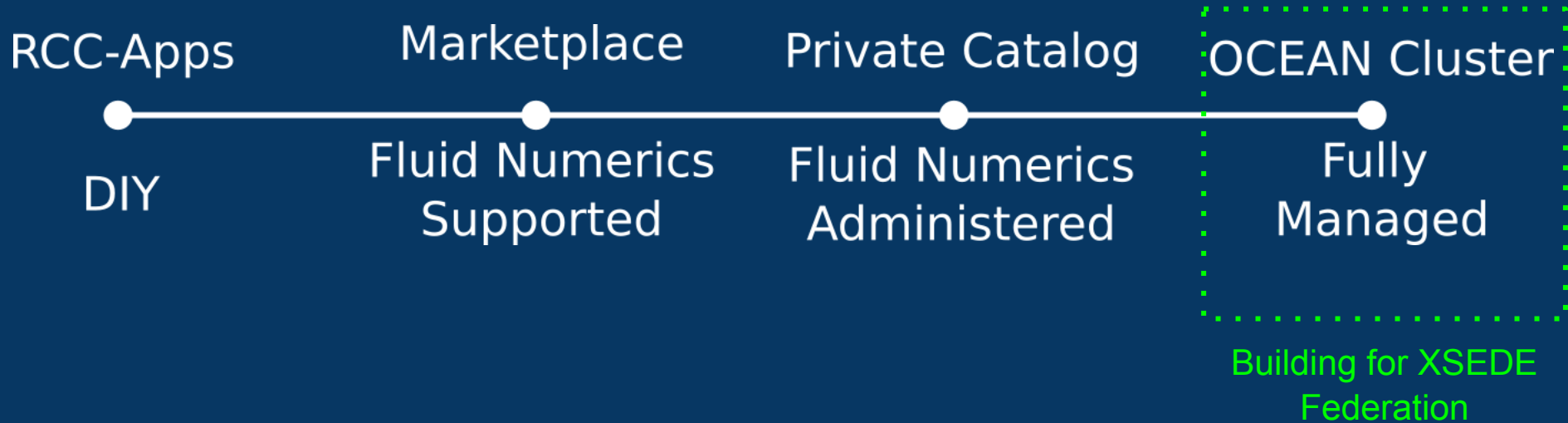
Developed and Maintained Resources

- VM Images
 - RCC Cluster (CentOS, Debian, Ubuntu)
 - Lustre
 - Application optimized VM Images
 - WRF, Gromacs, OpenFOAM, Paraview
- “Cluster-Services” System Support Scripts
 - Modify compute partitions, system mounts, and Slurm configurations on-the-fly
- Infrastructure-as-Code
 - Terraform modules for RCC Cluster and Lustre File System
 - Example ready-to-use deployments

RCC Image Dependencies



Research Computing Cloud



DIY Open-Source

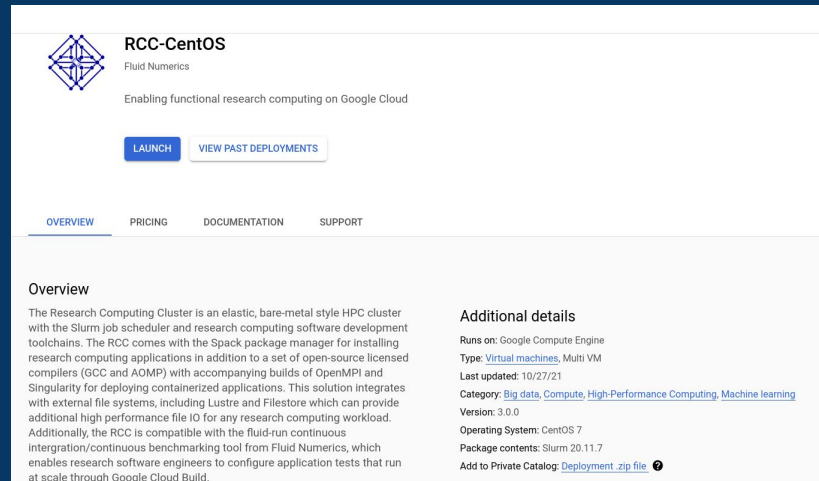
- RCC-Apps : <https://github.com/fluidnumerics/rcc-apps>
 - Create your own VM Images
- RCC-tf : <https://github.com/FluidNumerics/rcc-tf>
 - Deploy your cluster with Terraform infrastructure as code
- Lustre-GCP : https://github.com/FluidNumerics/lustre-gcp_terraform
 - Deploy a Lustre file system with Terraform infrastructure as code

Supported Solutions

Google Cloud Marketplace Licensed Images

- Click-to-deploy from Marketplace
- Terraform

<https://github.com/FluidNumerics/research-computing-cluster>



The screenshot shows the Google Cloud Marketplace page for the 'RCC-CentOS' image. The page features a logo for Fluid Numerics, a description of the image as 'Enabling functional research computing on Google Cloud', and buttons for 'LAUNCH' and 'VIEW PAST DEPLOYMENTS'. Below this is a navigation bar with links for 'OVERVIEW', 'PRICING', 'DOCUMENTATION', and 'SUPPORT'. The 'OVERVIEW' section is active, displaying a detailed description of the Research Computing Cluster as an elastic, bare-metal style HPC cluster. It also includes a section for 'Additional details' with metadata such as 'Runs on: Google Compute Engine', 'Type: Virtual machines, Multi VM', 'Last updated: 10/27/21', 'Category: Big data, Compute, High-Performance Computing, Machine learning', 'Version: 3.0.0', 'Operating System: CentOS 7', 'Package contents: Slurm 20.11.7', and 'Add to Private Catalog: Deployment .zip file'.

RCC-CentOS
Fluid Numerics
Enabling functional research computing on Google Cloud

[LAUNCH](#) [VIEW PAST DEPLOYMENTS](#)

[OVERVIEW](#) [PRICING](#) [DOCUMENTATION](#) [SUPPORT](#)

Overview

The Research Computing Cluster is an elastic, bare-metal style HPC cluster with the Slurm job scheduler and research computing software development toolchains. The RCC comes with the Spack package manager for installing research computing applications in addition to a set of open-source licensed compilers (GCC and AOMP) with accompanying builds of OpenMPI and Singularity for deploying containerized applications. This solution integrates with external file systems, including Lustre and Filestore which can provide additional high performance file IO for any research computing workload. Additionally, the RCC is compatible with the fluid-run continuous integration/continuous benchmarking tool from Fluid Numerics, which enables research software engineers to configure application tests that run at scale through Google Cloud Build.

Additional details

Runs on: Google Compute Engine
Type: [Virtual machines](#), Multi VM
Last updated: 10/27/21
Category: [Big data](#), [Compute](#), [High-Performance Computing](#), [Machine learning](#)
Version: 3.0.0
Operating System: CentOS 7
Package contents: Slurm 20.11.7
Add to Private Catalog: [Deployment .zip file](#)

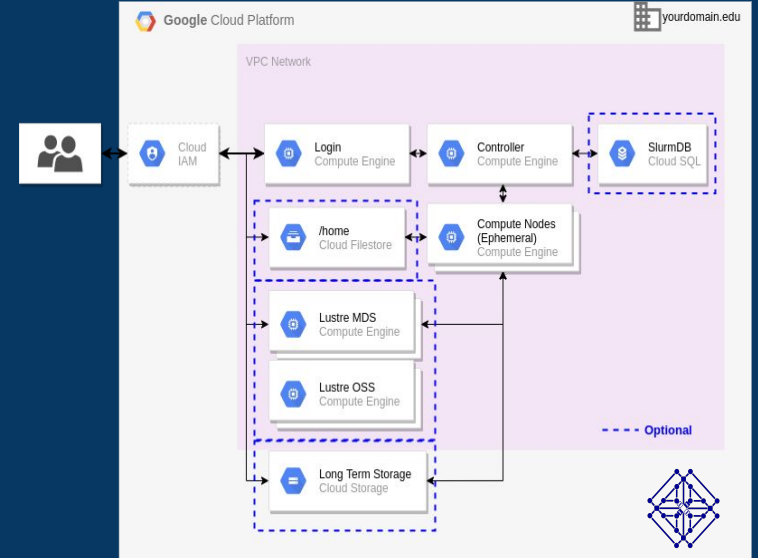
OCEAN Cluster

- Fiscally hosted by NPO branch of Fluid Numerics “WATERCHaNGE”
- Budget Transparency through Open Collective
 - <https://opencollective.com/waterchange>
 - <https://opencollective.com/oshackathon>
- Managed, Administered, and Supported by Fluid Numerics

OCEAN Cluster

Static Resources

- Login Node
- Slurm Controller
- Cloud SQL (Slurm Database)
- 2 TB Filestore (/home)



Lustre file-systems available when needed (15 minutes to provision)

OCEAN Cluster

Compute

- Intel Cascade Lake
 - 60 vCPU + 240 GB RAM per node
 - Quota Maintained : 10 Node per region
- Intel Cascade Lake + Nvidia A100 GPU
 - Configurable, up to 96 vCPU + 16 GPU per node
 - Quota Maintained : 80 A100 GPU per region
- Intel Broadwell + Nvidia V100 GPU
 - Configurable, up to 96 vCPU + 8 GPU per node
 - Quota Maintained : 50 V100 GPU (us-west1) and 8 V100 GPU per region elsewhere
- Intel Broadwell + Nvidia P100 GPU
 - Configurable, up to 96 vCPU + 8 GPU per node
 - Quota Maintained : 50 V100 GPU (us-west1) and 8 P100 GPU per region elsewhere
- AMD EPYC Rome
 - 224 vCPU + 896 GB RAM per node
 - Quota Maintained : 2 Node per region

Additional Compute (Upon Request)

- Intel Broadwell + Nvidia P4
- Intel Broadwell + Nvidia T4

System size can be increased given demand and acceptance of Quota Request

OCEAN Cluster

Compilers, MPI, & Container Platforms

- GCC 9.2.0, 10.3.0, 11.2.0
- AMDFlang/Clang
- Intel OneAPI Compilers
- OpenMPI 4.0.2
- Singularity 3.7.4

Developer Tools

- ROCm
- CUDA
- Intel Advisor, VTune, & Thread Inspector
- HPC Toolkit
- DMTCP (Checkpointing & Restarting)

COVID-19 HPC Consortium

Dr. Suchetana Gupta (Indian Institute for the Cultivation of Science)

- Two series of Google Cloud Research credits (\$7K/each)
- Custom VM Image builds for AMBER
 - Build scripts available at <https://github.com/FluidNumerics/rcc-apps/tree/main/amber>
- Provided Technical Support for Slurm and Google Cloud

Resulting Publications

Gupta, Suchetana & Mallick, Ditipriya & Banerjee, Kumarjeet & Sarkar, Soumyadev & Lee, Sonny & Basuchowdhuri, Partha & Jana, Siddhartha. (2021). D155Y Substitution of SARS-CoV-2 ORF3a Weakens Binding with Caveolin-1: An in silico Study. 10.1101/2021.03.26.437194.

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