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
  ○ WATERCHA.NGE 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
Research Computing Cloud

RCC-Apps

DIY

Marketplace

Fluid Numerics Supported

Private Catalog

Fluid Numerics Administered

OCEAN Cluster

Fully Managed

Building for XSEDE Federation
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
OCEAN Cluster

- Fiscally hosted by NPO branch of Fluid Numerics “WATERCHaNGE”

- Budget Transparency through Open Collective
  - [https://opencollective.com/waterchange](https://opencollective.com/waterchange)
  - [https://opencollective.com/oshackathon](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

Fluid Numerics

Research Computing Cloud
XSEDE