Prove-of-concept:
Cycling Data Assimilation Workflows in the Cloud

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Motivation:
Cloud-Based Reanalyses and Reforecasts (R&R)

Offload Reanalysis and Reforecasts from NOAA’s on-prem HPC:

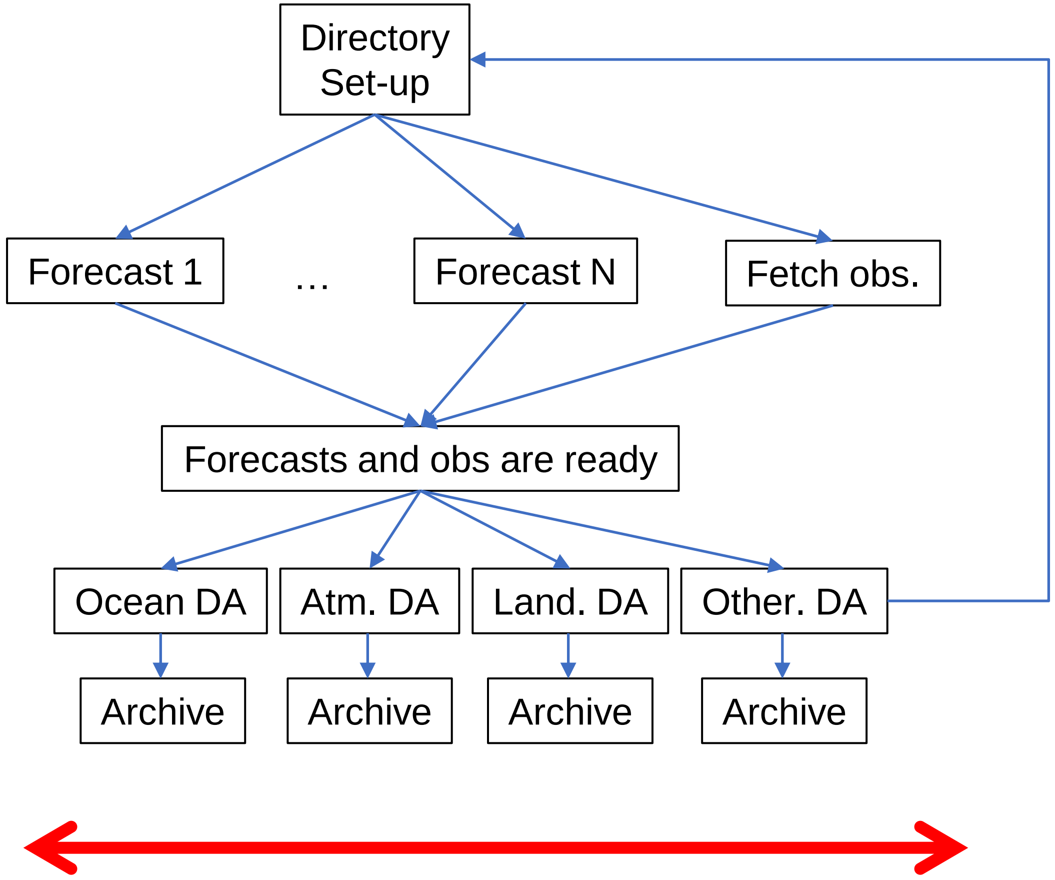
- Insufficient capacity of NOAA on-prem to transition research to operations;
- 30 yrs of ensemble R&R required for major GEFS upgrades;
- GEFS v12 RNR took 2 years at lower resolution of atmosphere-only;
- GEFS v13 RNR will be higher-res and will be atmosphere/ocean/land/sea-ice.

Enable Community Collaboration:

- Make NOAA datasets available for community to enable post-processing and tuning efforts.
- Provide R&R software stack to the community outside NOAA’s restrictive secured network.

Workflow footprint

Target:
High-resolution (1/4°) with ensemble



Directory Set-up

Forecast 1

…

Forecast N

Fetch obs.

Forecasts and obs are ready

Ocean DA

Atm. DA

Land. DA

Other. DA

Archive

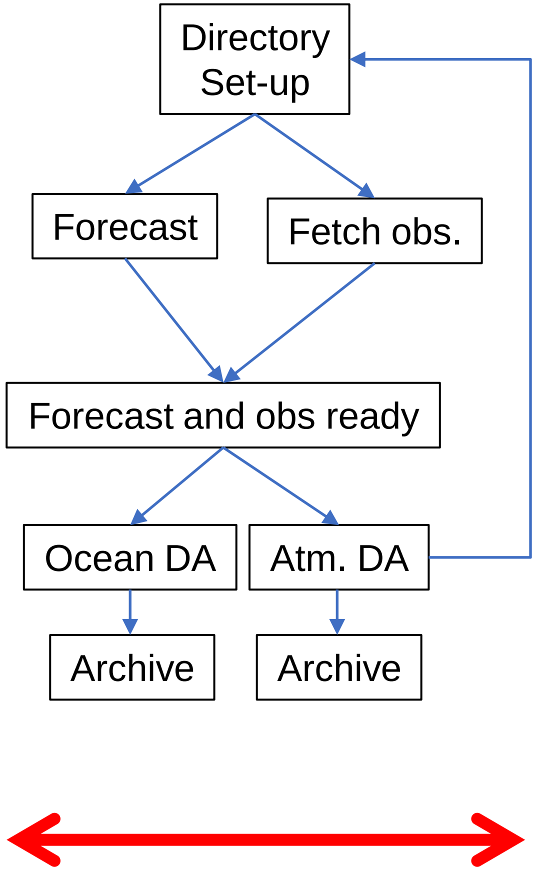
Archive

Archive

Archive

5K-30K CPU cores

Prototype (this presentation):
Low-resolution (1°) deterministic



Directory Set-up

Forecast

Fetch obs.

Forecast and obs ready

Ocean DA

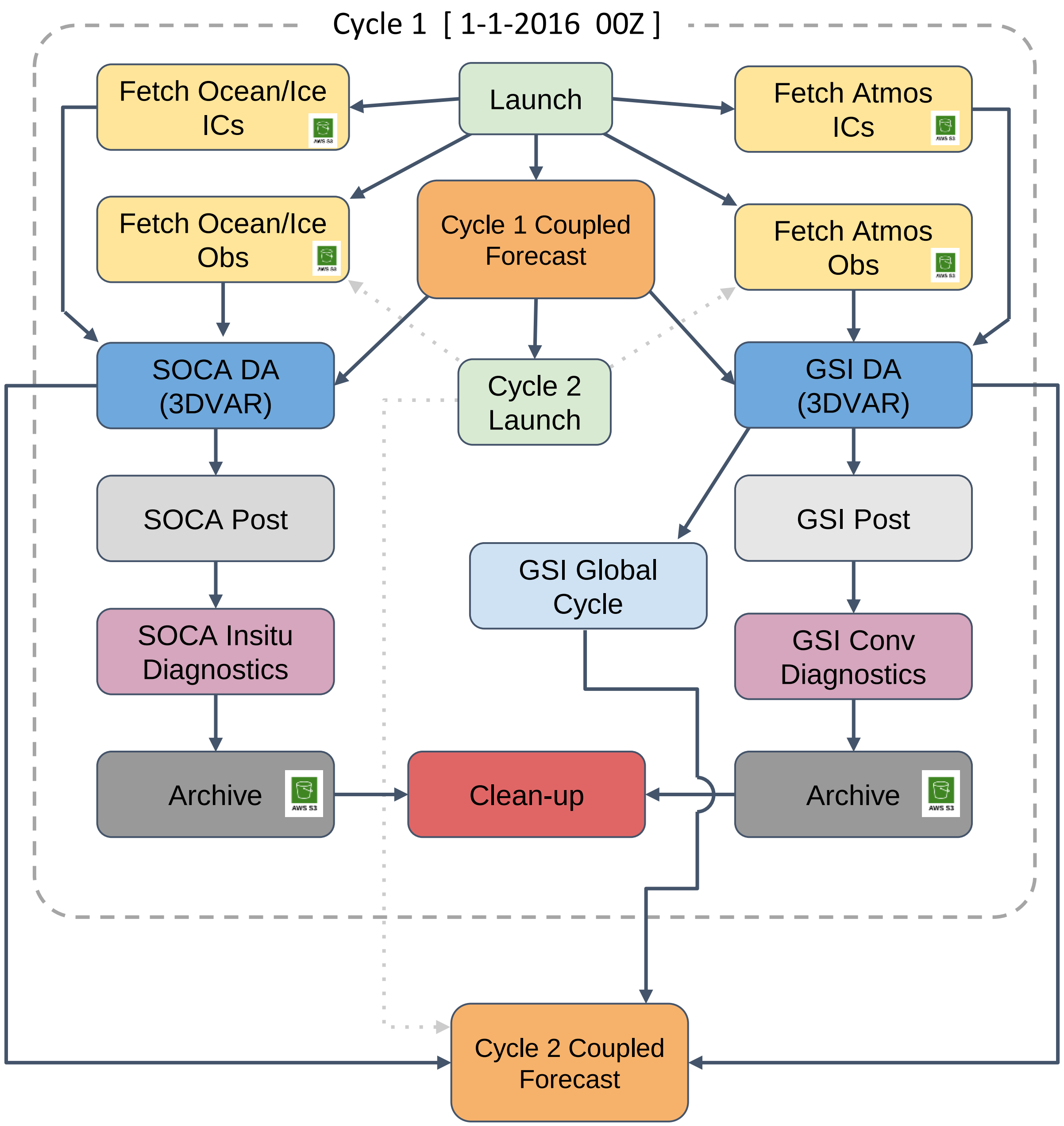
Atm. DA

Archive

Archive

~200 CPU cores

Prototype 3DVAR Workflow



Cycle 1 [1-1-2016 00Z]

Fetch Ocean/Ice ICs

Launch

Fetch Atmos ICs

Fetch Ocean/Ice Obs

Cycle 1 Coupled Forecast

Fetch Atmos Obs

SOCA DA (3DVAR)

Cycle 2 Launch

GSI DA (3DVAR)

SOCA Post

GSI Post

GSI Global Cycle

SOCA Insitu Diagnostics

GSI Conv Diagnostics

Archive

Clean-up

Archive

Cycle 2 Coupled Forecast

Task	CPU	MEM	IO	MPI Threads
Critical Tasks (must successfully run each cycle)				
Launch	Low	Low	Low	1
Fetch Atmos ICs Fetch Ocean/Ice ICs Fetch Atmos Obs Fetch Ocean/Ice Obs	Low	Low	High	1
Coupled Forecast	High	High	High	208
GSI DA (3DVAR) SOCA DA (3DVAR)	High	Very High	High	80
GSI Global Cycle	High	Med	Med	6
Non-Critical Tasks (can fail without affecting results)				
GSI Post SOCA Post	Low	High	High	1
GSI Conv Diagnostics SOCA Insitu Diagnostics	Med	Med	Med	1
Archive	Low	Low	High	1
Clean-up	Low	Low	Low	1

General Cloud Implementation Considerations

High Level Architecture

- Replicate on-premises setup (workflow runs as close to on-prem HPC as possible)
- Stage as much input data on blob storage as possible (S3 or Azure Block Blob)
  - Push initial conditions (IC) and observation data (Obs) to NOAA Big Data Program (BDP) with free egress
  - Use BDP for both On-Prem and Cloud cycling systems (much faster than On-Prem tape storage)
- Hybrid setup (some apps containerized - some apps natively compiled)
- Use Cylc workflow manager
- Use Slurm manager to acquire compute resources
- Except for resource configuration, On-Prem HPC workflow is identical to Cloud Workflow

Component Choices

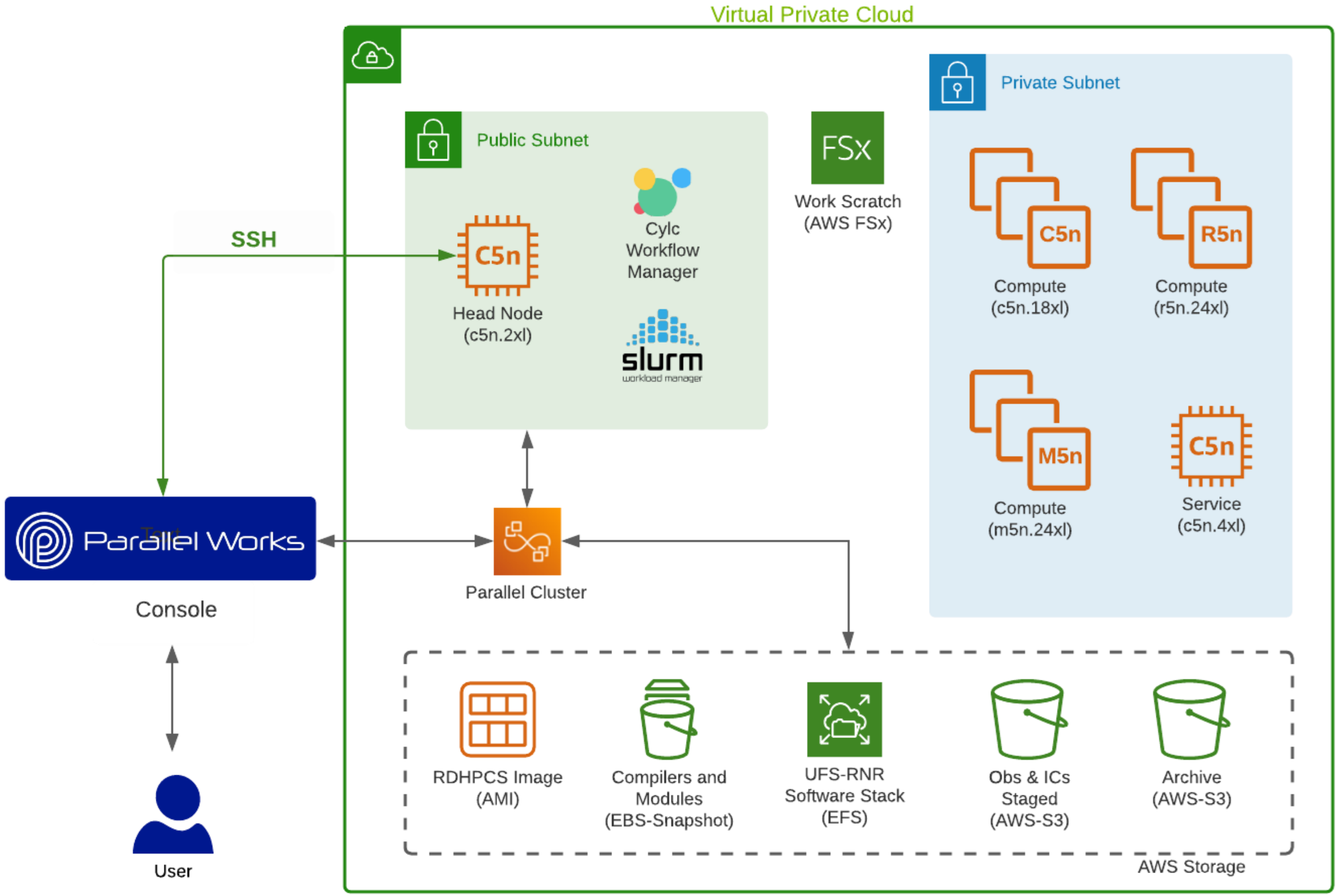
- Compute instance types:
  - Network optimized: AWS - efa, Azure - Infiniband
  - AWS: Trade-off between compute and memory - C5n, R5n, M5n
  - AZURE: HPC optimized - hc44rs
  - AMD™ or Intel™ : On-Prem compile is optimized for Intel
- Scratch Storage:
  - Lustre
  - Network storage: AWS EBS, AZURE NetAPP
  - Local disk: Azure BeeOND
- Data and software stack location:
  - AWS: EBS or EFS
  - Azure: Block Blob or nfs 3.0

Access to Cloud Platforms

- Direct access: AWS vs Azure
  - More service options but also more setup work

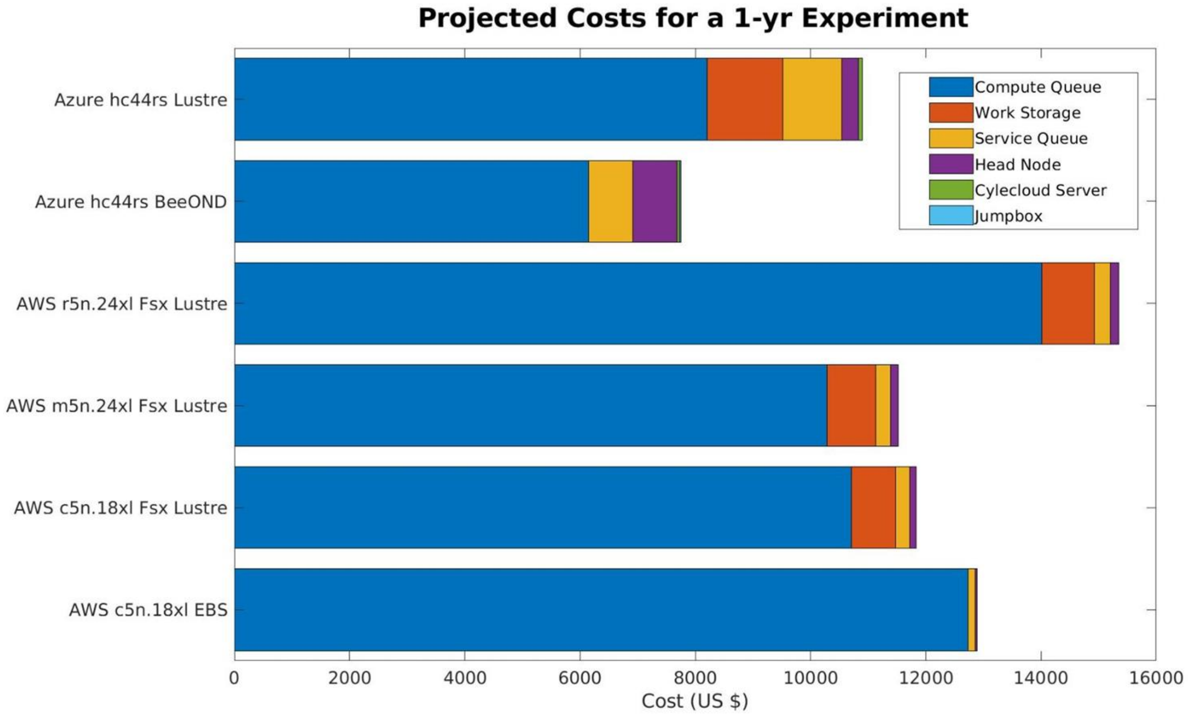
- ParallelWorks : multi-cloud platform for AWS, Azure, GCP
  - Rapidly evolving and relatively young platform
  - Easy cluster deployment (caveat - only after fair amount of initial setup)
  - No custom instance images allowed
  - Restricted subset of configurations for node and service management

AWS ParallelWorks Account
Cloud Architecture



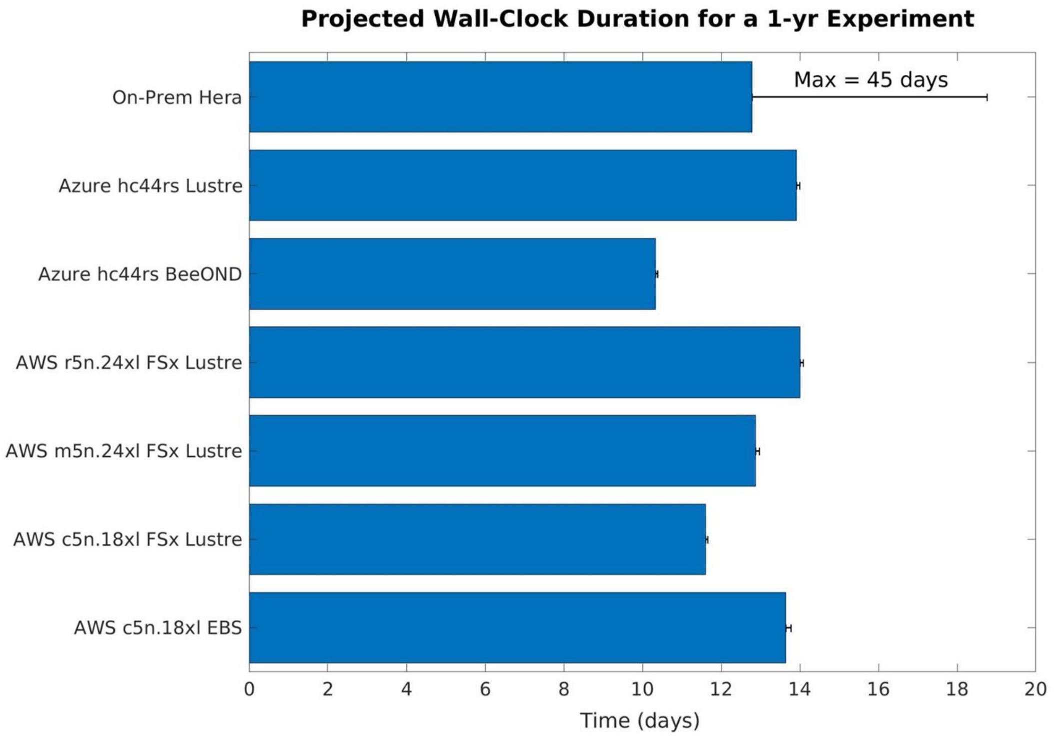
AWS Parallel Cluster™:	create and manage cluster
Master node (c5n.2xl):	compiling, cylc, slurm, NFS mounts
Compute queues:	compute - c5n.18xl big-mem - r5n.24xl generic - m5n.24xl service - c5n.4xl
Luster service (FSx):	classic work scratch
Persistent storage:	s3 for staged input data - ICs and Obs
Software stack:	OS - Alinux2 (CentOS compatible) PW stack - compiler, MPI Application - RnR

Cost Comparisons



- Compute costs dominate on all platforms
- Lustre: costly but can be configured to be cheaper
- Azure requires more vm overhead (cyclecloud) but instances are slightly cheaper per hour
- BeeOND: faster and free but not fault tolerant
- Using generic mode with EFA (m5n) was more cost effective than compute-optimized or memory-optimized nodes.

Throughput Comparisons



- On-Prem can be fast and is already budgeted, but in practice resource competition between researchers can degrade throughput substantially
- All Cloud platforms show consistent and predictable throughput that is comparable or faster than On-Prem

Lessons learned

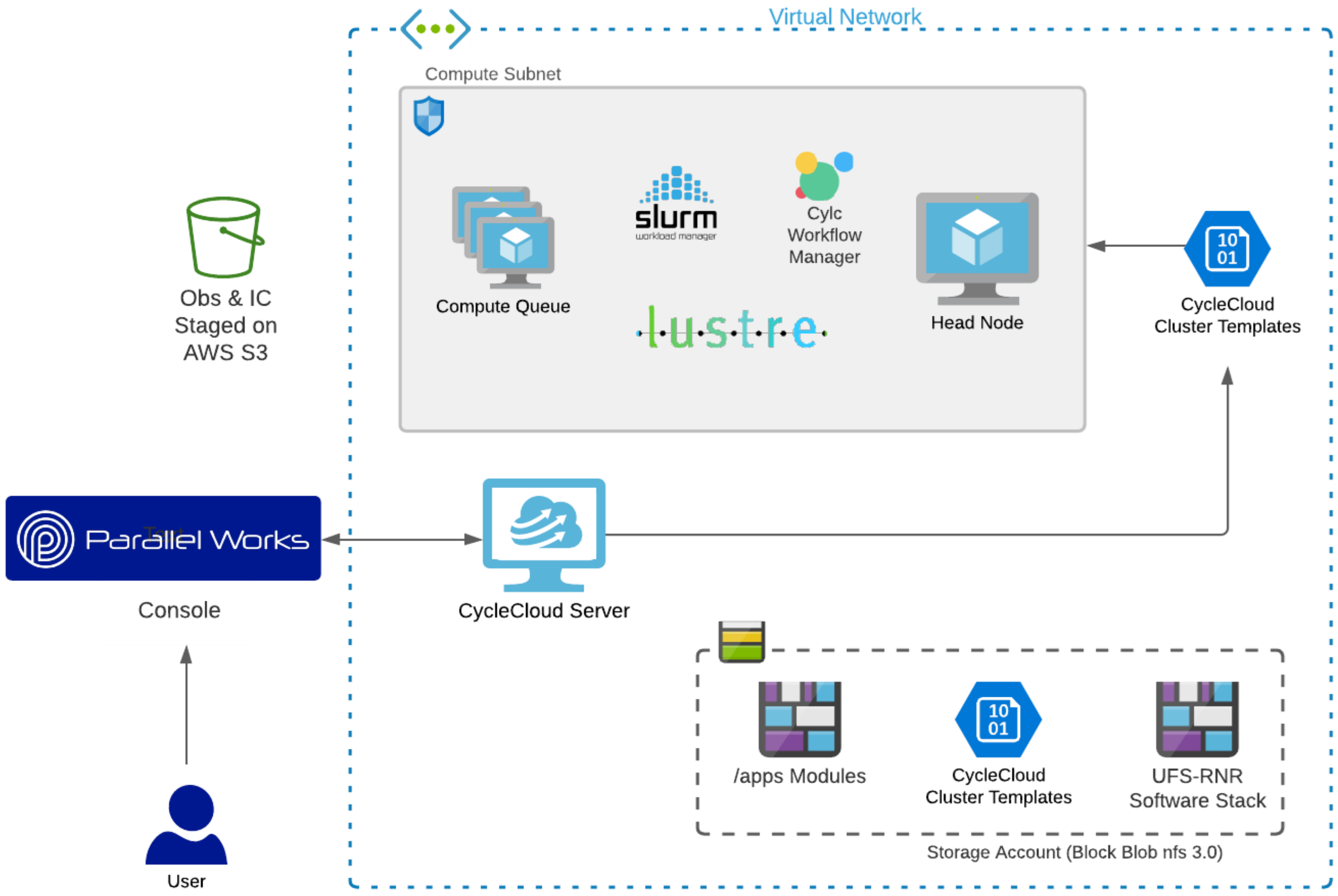
- Fast interconnect is essential for DA workflow (e.g. DA solvers);
- Scaling compute footprint up and down is impractical in cycling workflow;
- Memory-optimized nodes are expensive;
- Storage choices affect performance and cost;
- Containers are tricky for multi-node MPI jobs;
- Spot availability is spotty (at least on AWS)
- Compiling natively can be time-consuming (but we were successful at using binaries compiled on Azure to run on AWS)

Conclusions from Cloud Testing

- Scientific results indistinguishable from On-Prem.
- Cost of the scaled-down workflow is affordable.
- Throughput matches or beats practical On-Prem performance.
- Hybrid (CSP/on-prem) deployments are possible:
  - E.g. can run reanalyses streams using combination of on-prem and CSP.
- Next steps:
  - Run extensive simulations (multiple decades);
  - Explore using spot computing on Azure;
  - Develop cloud-enabled diagnostic capabilities.

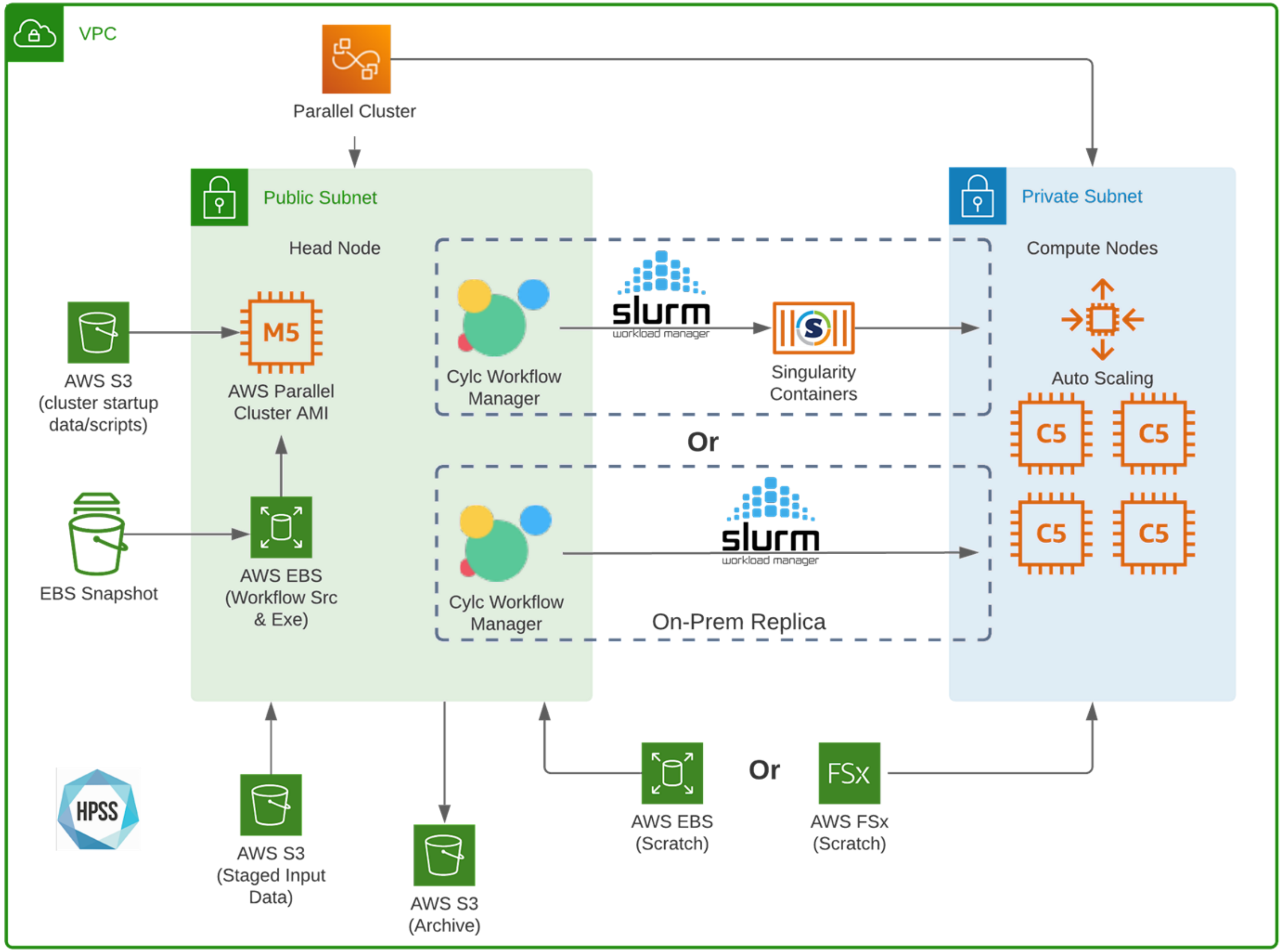
End

Parallel Works Managed Azure Cloud Architecture

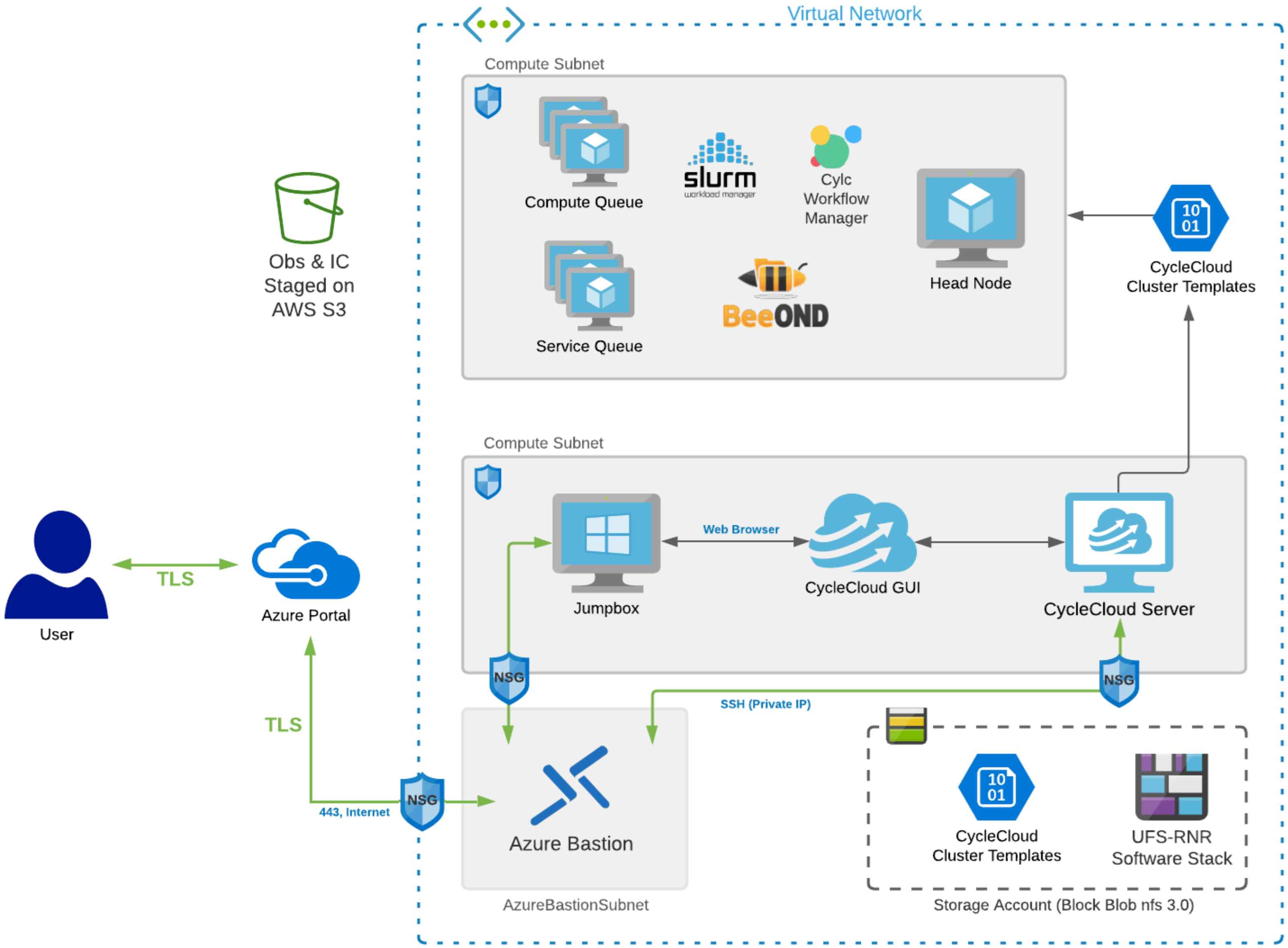


Azure CycleCloud™:	create and manage cluster
Master node (h8):	compiling, cylc, slurm, NFS mounts
Compute queue (hc44rs):	balanced compute and memory
Luster cluster (D8ds_v4):	1 mds node and 2 oss nodes - classic work scratch
Persistent storage (aws s3):	staged input data (ICs and Obs)
Software stack (block blob):	OS - CentOS 7, PW stack (compiler, MPI), application (RnR) on block blob nfs 3.0 storage.

AWS OAR-TigerTeam Account Cloud Architecture

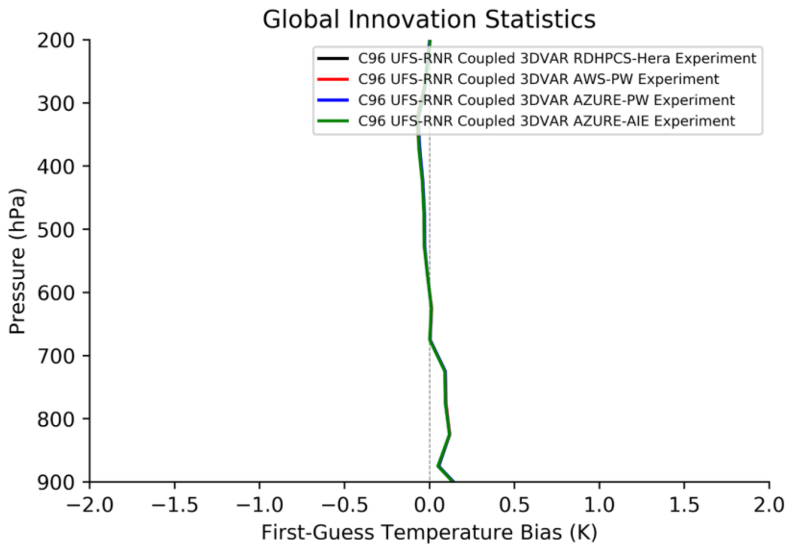


MS Azure AI for Earth Account Cloud Architecture

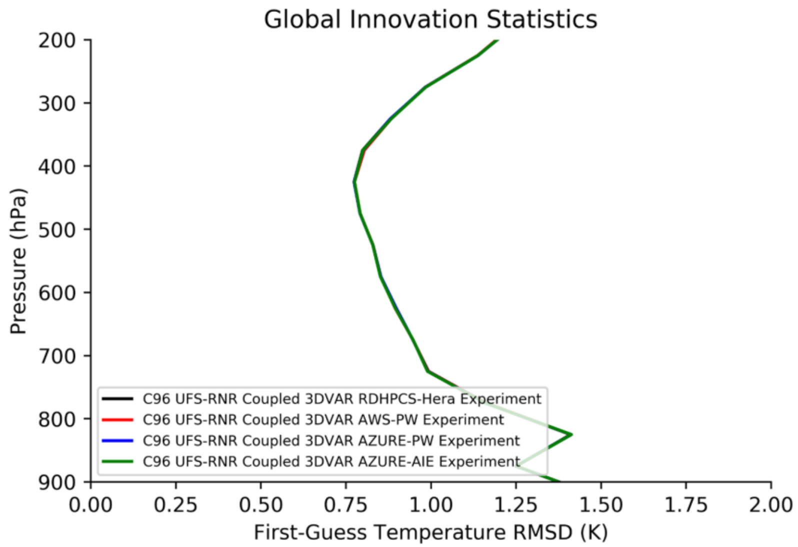


Cloud-Based Workflow Is Scientifically Accurate

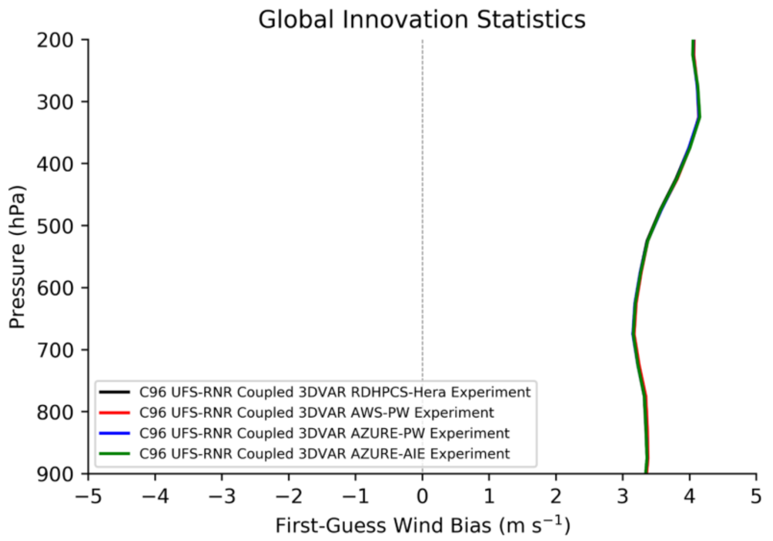
15-day Experiment Starting on 1-1-2016 (Cloud Matches Hera)



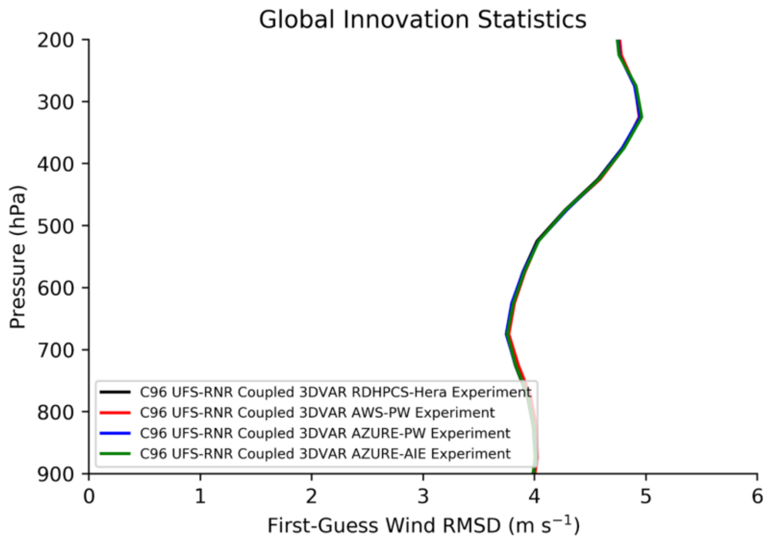
Global Innovation Statistics



Global Innovation Statistics

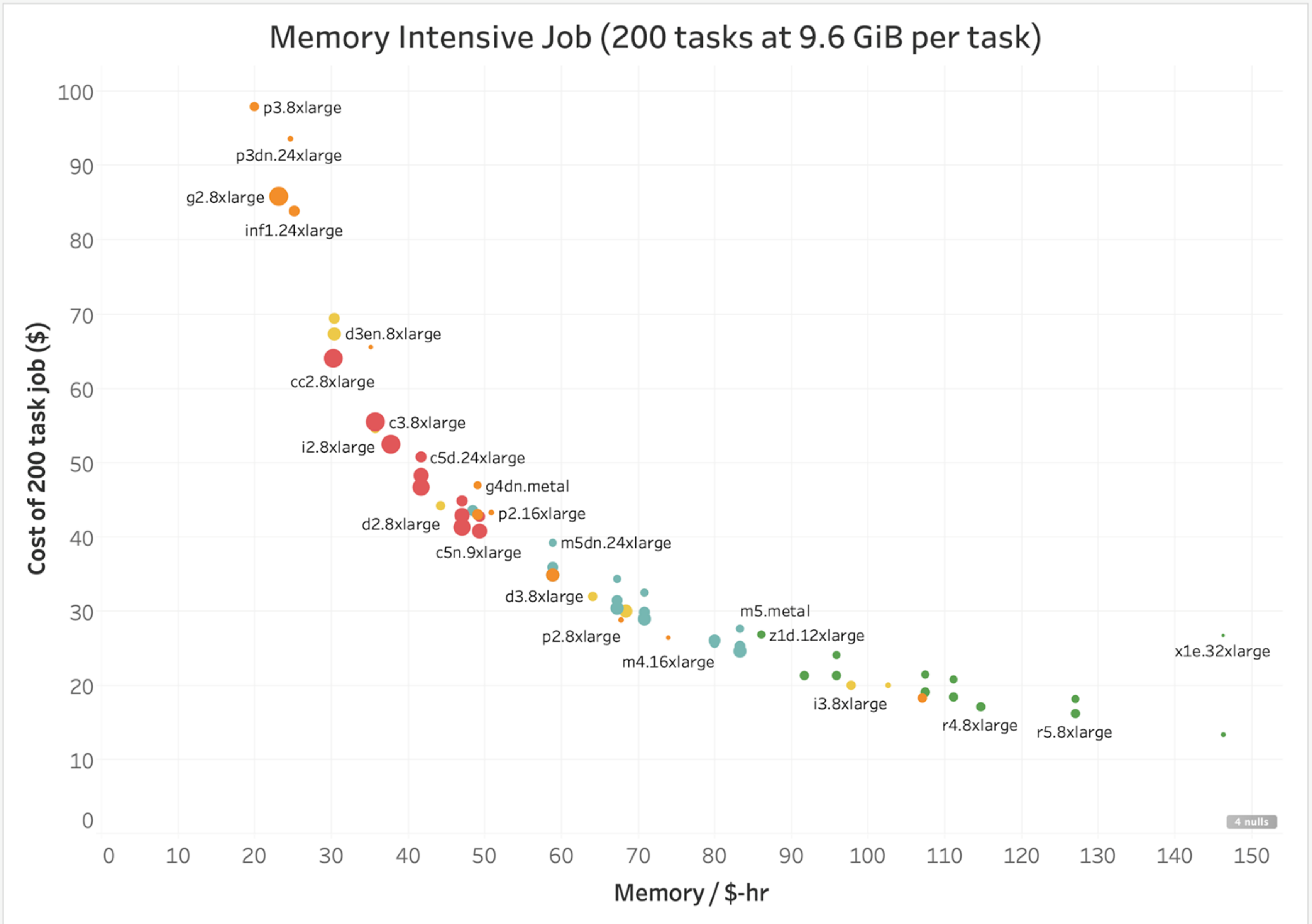


Global Innovation Statistics



Global Innovation Statistics

AWS Elastic Compute Cloud (EC2)
Instance Type / Capacity Considerations



Balance

- Capability
- Availability
- Cost

Instance Family

🟧 Accelerated Computing

🟥 Compute Optimized

🟦 General Purpose

🟩 Memory Optimized

🟨 Storage Optimized

Nodes Required

● 1.00

● 10.00

● 20.00

● 33.00