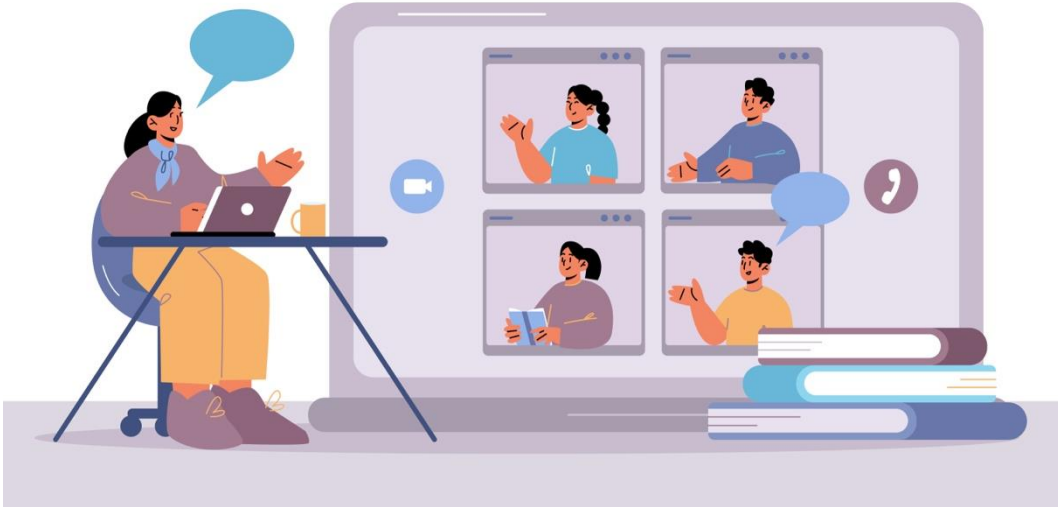


Community Modeling and Analyses (CMAS) Center Webinar Series



25 years of Serving a Global Community

CMAS Center Trainings



- Spring 2026
 - SMOKE Online, April 7 – 10
 - CMAQ Online, April 21 – 24
- Fall 2026
 - SMOKE Online, October 13 – 16
 - CMAQ Online, October 27 – 30

**** Seats available. Register soon ****

<https://cmascenter.org/training/classes.cfm>

25th Annual CMAS Conference



Chapel Hill, NC

October 19–21

Look out for Call for Abstracts and announcements coming soon!

<https://cmascenter.org/conference/2026/index.cfm>

CMAQ on the Cloud Help Sessions



CMAQ on the Cloud – Monthly Zoom Help Session

Hosted by: CMAS Center @ UNC

Audience: Modelers exploring or running **CMAQ on the Cloud**

Goal: Provide one-on-one support to members of the CMAS community

Topics Covered

- Troubleshooting AWS or Azure cloud **HPC resource provisioning**
- **Benchmarking CMAQ v5.4** (2018 12US1 2-day domain) on cloud HPC clusters
- Accessing input data & archiving outputs using **S3 copy** or **Lustre *lazy loading*** from the **CMAS Data Warehouse (AWS Open Data Registry)**
- Using **BeeGFS on Microsoft Azure CycleCloud**

When: **First Thursday of every month, 3 – 4 PM ET**

Upcoming Sessions: Apr 2 • May 7 • Jun 4 • Jul 2

Upcoming CMAS Webinar: Exploring AMET Web on AWS



Save the Date: Thursday May 14 1:00 – 2:30 ET

- **Next CMAS Webinar on May 14 to demonstrate AMET Web on single VM**
 - **Interactive web-based approach to use AMET for model evaluation on the Cloud (Will include a Live Demo)**
- Documentation:
 - AMET AQ Website:
https://pcluster-cmaq.readthedocs.io/en/latest/user_guide_pcluster/amet/ami_website.html#create-air-quality-plots-using-the-amet-aq-website
 - AMET MET Website:
https://pcluster-cmaq.readthedocs.io/en/latest/user_guide_pcluster/amet/ami_website.html#create-met-plots-using-the-amet-met-website

03/19/2026

Lessons Learned for Performing Long-Term CMAQ Production Simulations for the 12US1 and 36US3 Domains on AWS Parallel Cluster

Manish Soni, Elizabeth Adams and Saravanan Arunachalam

UNC Institute for the Environment | CMAS Webinar



The University
of North Carolina
at Chapel Hill

Outline



- Motivation
- CMAQ Modeling Framework and Study Domains
- AWS ParallelCluster Architecture
- Benchmark Setup
- Performance Results
- Storage and Cost Optimization
- Lessons Learned
- Recommended Configuration
- Future Work

Motivation



- Long-term CMAQ simulations require **significant HPC resources**
 - Air quality metrics for regulatory applications or quantifying health impacts and climate interactions need annual or even multi-annual simulations
- Cloud computing enables **scalable HPC environments**
- AWS ParallelCluster simplifies **cluster deployment**

Problem Statement

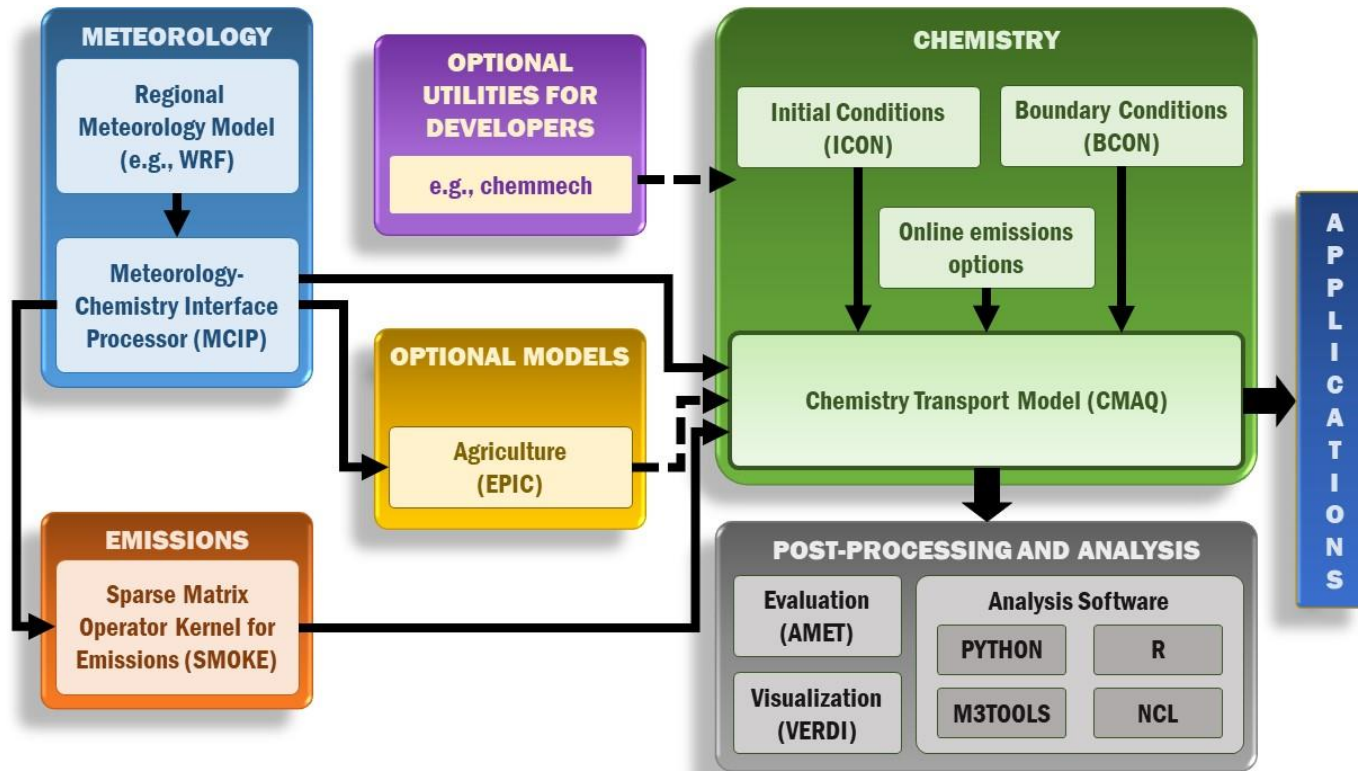


- Traditional HPC clusters have **limited availability and fixed capacity**
- Cloud computing provides **on-demand scalable resources**
- However, **cost and performance tradeoffs must be evaluated**

Objectives

- Identify **cost-efficient AWS configuration for CMAQ production runs**
- Perform **long-term CMAQ simulations** on AWS Parallel Cluster and provide guidance for CMAS community

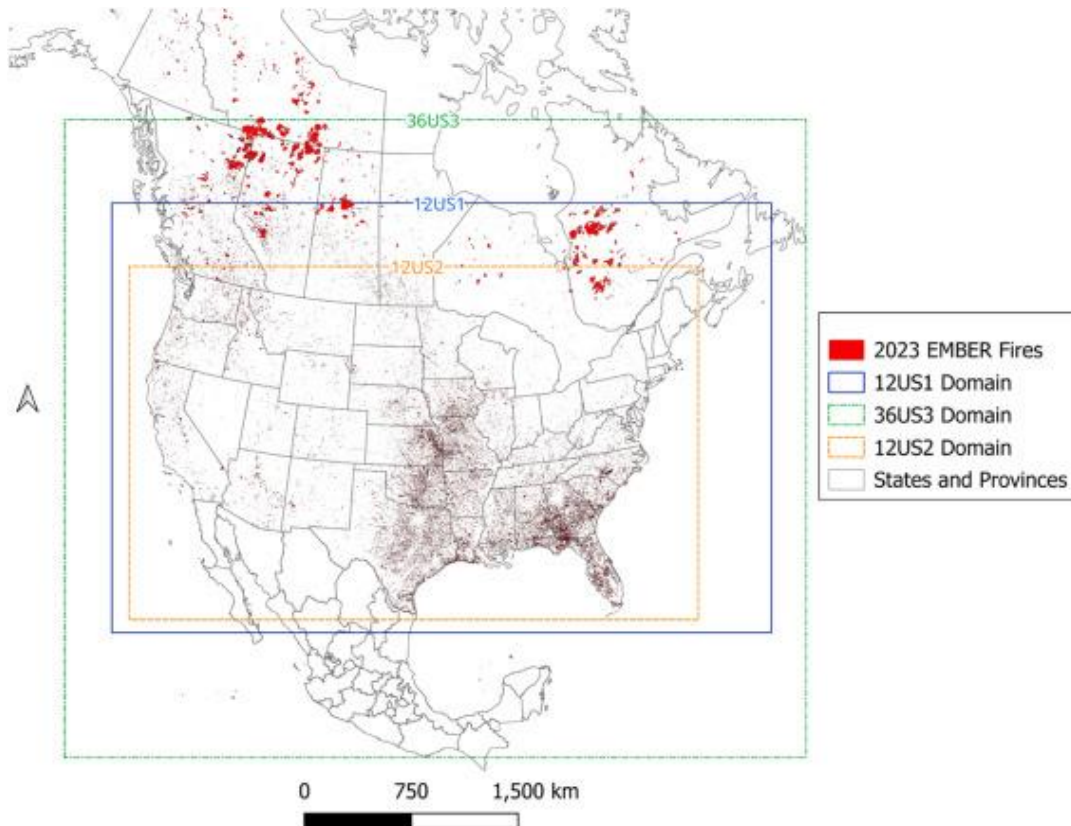
CMAQ Modeling System Framework



- Community Multiscale Air Quality Model (CMAQ) simulates O_3 , $PM_{2.5}$ and NO_2 , etc. for different air quality applications
- Requires large-scale HPC resources
- Typical production runs require annual simulations

Source : <https://www.epa.gov/cmaq/cmaqs-purpose>

Domains Used in Study



- **12US1 domain:** 499×259
(columns \times rows)
- **36US3 domain:** 172×148
- Used for **benchmarking computational costs**
- **Different compute and storage requirements**

Source: Simon, H et al., (2025). Expedited modeling of burn events results (EMBER): A screening-level dataset of 2023 ozone fire impacts in the US. *Data in Brief*, 58, 111208.

Running on Single Virtual Machine (VM) vs Parallel Cluster



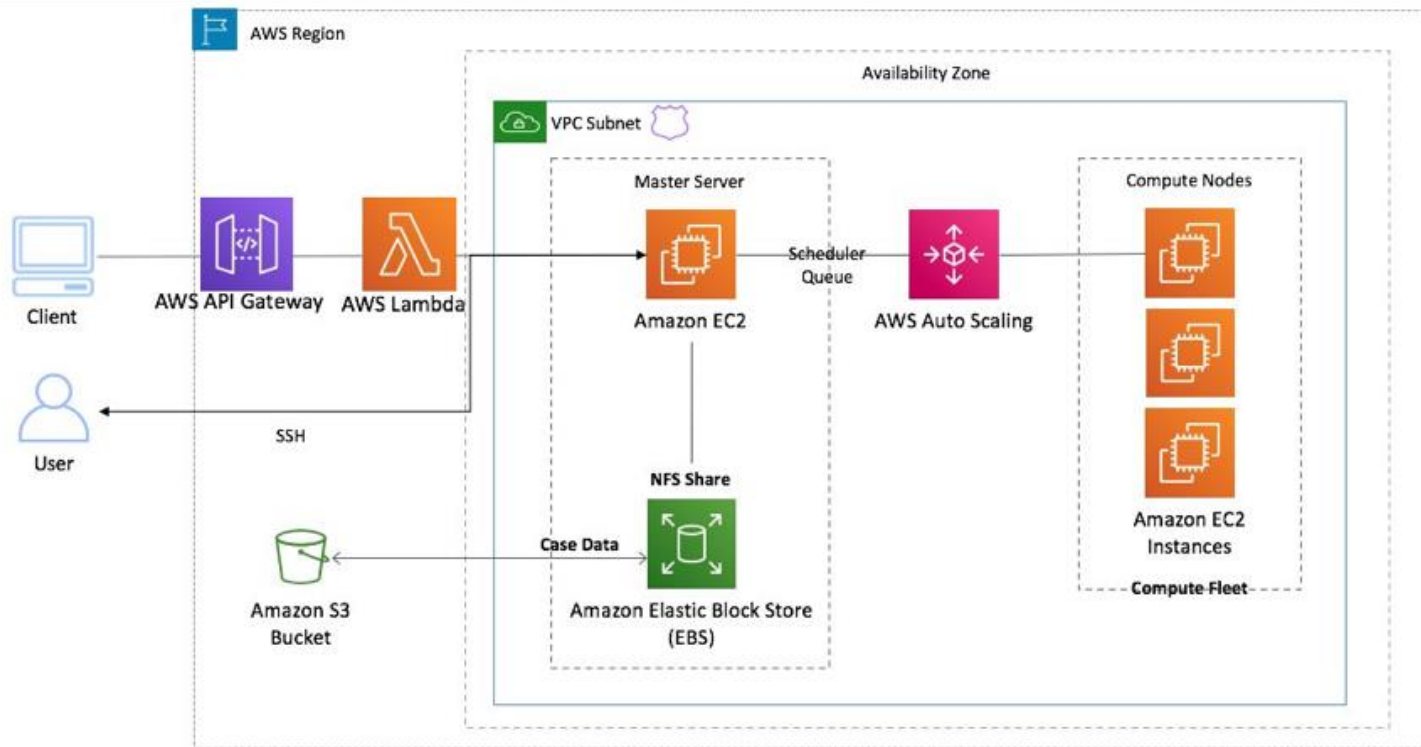
- **Single VM:** A single virtual machine with fixed CPU, memory, and storage where tasks run on one node. It is simple to set up but limited in scalability and performance
- **ParallelCluster:** A group of multiple interconnected machines (nodes) that work together to execute tasks simultaneously. It provides higher performance, scalability, and is suitable for large-scale simulations or HPC workloads
- Example
 - **Single VM:** Running a CMAQ simulation on one EC2 instance
 - **Parallel Cluster:** Running CMAQ across multiple nodes using MPI with a fast interconnect like **AWS Elastic Fabric Adapter** (network interface for faster intercommunication within nodes)



Prerequisite for AWS parallel Cluster

- **AWS Account** with billing enabled and access to the AWS Management Console
- **IAM permissions** to create and manage AWS resources (EC2, VPC, FSx, S3, Auto Scaling)
- **AWS CLI installed and configured** to interact with AWS services from the command line
- **Python environment (Python 3.8 or later)** to install and run ParallelCluster tools
- **EC2 Key Pair** for secure SSH access to the cluster head node
- **VPC networking setup** including subnets, security groups, and internet gateway
- **HPC EC2 instances** (e.g., **hpc7g** or **hpc6a**) for high-performance parallel workloads
- **Shared storage configuration** such as **FSx for Lustre** for fast parallel file access
- **Amazon S3 storage** for input data, output results, and backups (optional)

AWS ParallelCluster Architecture



- Open-source tool for deploying HPC clusters on AWS
- Supports SLURM workload manager
- Automates cluster creation and scaling
- SLURM dynamically provisions the compute nodes and deregisters them once the job is complete, ensuring that compute costs are only incurring costs during job execution
- Supports FSx for Lustre and EFA

Source :<https://aws.amazon.com/blogs/compute/using-aws-parallelcluster-with-a-serverless-api/>

AWS Parallel Cluster Storage and Networking



Elastic Block Storage (EBS)

Configure to use maximum Input/Output Operations per Second (IOPS) and throughput. EBS allows users to provision performance independent of storage capacity

- High performance, low-latency disk

Lustre/FSx (used on ParallelCluster)

- Process massive datasets at up to hundreds of gigabytes per second of throughput, millions of IOPS, and sub-millisecond latencies
- Capable of “*lazy loading*” data (loading data when it is first used) from S3 bucket

Simple Storage Service (S3) (used on ParallelCluster)

Archive data at the lowest cost

- Run cloud-native applications by *lazy loading* from the s3 bucket to /fsx

Network Options used

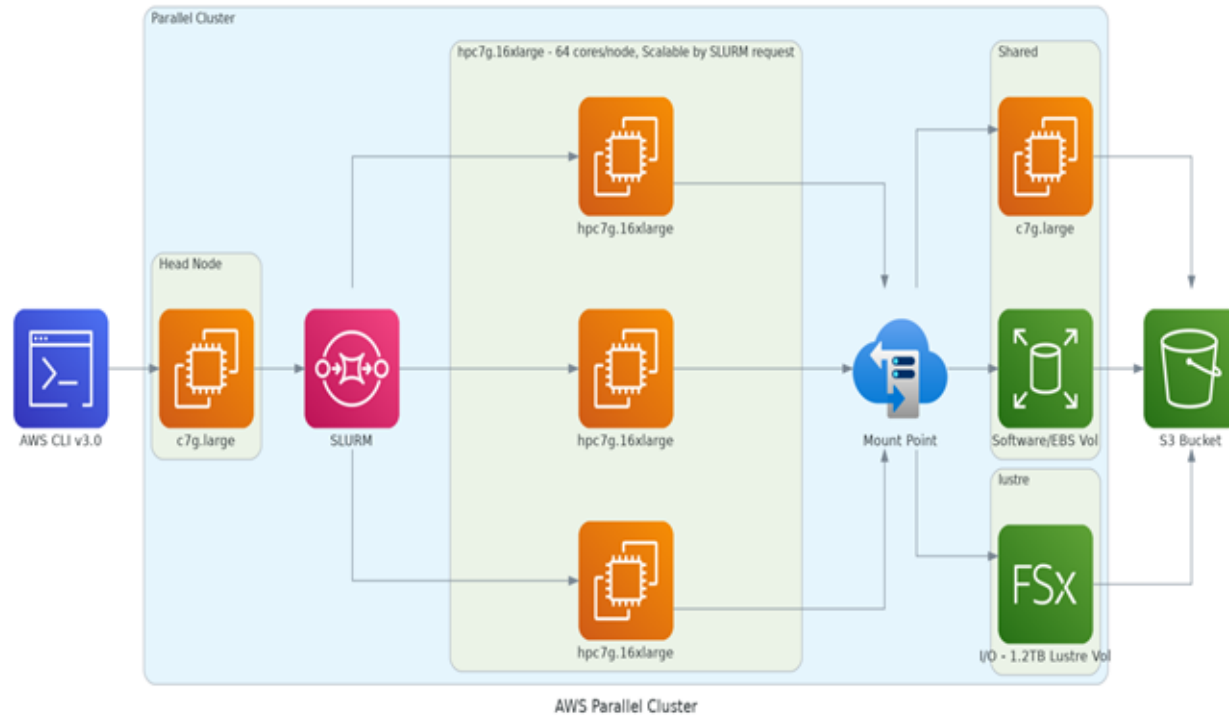
- Elastic Fabric Adapter (EFA) enabled
- High throughput

AWS Parellel Cluster Deployment



- Clusters deployed in US-East regions
- ARM64 cluster using Graviton3E processors
- x86_64 cluster using AMD EPYC processors
- Separate build environments created for benchmarking
- ARM64 does not support intel compilers
- Compilers installed on x86_64: intel 25.0.4 and gcc 11.4.1
- Compilers installed on ARM64: gcc 11.4.1
- Operating System: ubuntu
- Parallel cluster Version: 3.12

AWS ParallelCluster Architecture for CMAQ



Why HPC EC2 instances are required for CMAQ

- CMAQ requires **highly parallel HPC compute resources**
- Use **AWS HPC instances (hpc7g, hpc6a)**
- Built on **AWS Nitro System** for low-latency internode communication
 - **Up to 200 Gbps network bandwidth** for tightly coupled workloads
- Enables **highly scalable CMAQ simulations**

Architecture and Processor Selection



Component	x86_64 Cluster	ARM64 Cluster
Login Node	c6a.xlarge 4 cores 8GB RAM \$0.15/hour	c7g.large 2 cores 4GB RAM \$0.07/hour
Compute Node	hpc6a.48xlarge 96 cores 384 GB RAM \$2.88/hour	hpc7g.16xlarge 64 cores 128 GB RAM \$1.68/hour
Architecture	x86_64	ARM64
Region	us-east-2 (Ohio)	us-east-1 (N. Virginia)

Benchmark Methodology



- Initial tests conducted using **12US1 domain**
- Performance metric: Average **CPU-sec/day**
- **Different processor counts** evaluated
- **Shared** storage and **Lustre** storage tested
- CMAQ version : **5.4+**
- Mechanism : **cb6r5_ae7**
- Compilers : **intel/gcc**

AWS Parallel Cluster Workflow



1

Activate environment (python CLI) and Install Parallel cluster v 3.12
`source ~/hpc-ve/bin/activate`

2

Configure the cluster using with AWS CLI 3.0
`pcluster configure --config hpc7g.16xlarge.yaml`

3

Modify YAML to use CMAQ snapshot and Lustre storage

4

Create the ParallelCluster
`pcluster create-cluster --cluster-configuration hpc7g.16xlarge.yaml --cluster-name cmaq --region us-east-1`

5

Check cluster status
`pcluster describe-cluster --region=us-east-1 --cluster-name cmaq`

6

Connect to head node
`pcluster ssh -v -Y -i ~/cmasc.pem --region=us-east-1 --cluster-name cmaq`

7

Run CMAQ simulations
Submit jobs to SLURM queue and use Lustre for output

8

Delete Cluster
`pcluster delete-cluster --region=us-east-1 --cluster-name cmaq`

Complete Step by step method how to install and create Single VM and parallel cluster is available here:

https://pcluster-cmaq.readthedocs.io/en/latest/user_guide_pcluster/cmaq-vm/quick-start.html

Git repository for preconfigured yaml examples and run scripts to use for running CMAQ v5.4

<https://github.com/CMASCenter/pcluster-cmaq>

CMAS Data Warehouse



CMAS Data Warehouse on AWS is a CMAS-Center repository to disseminate meteorology, emissions, and air quality model input and output for Community Multiscale Air Quality (CMAQ) Model Applications

<https://registry.opendata.aws/cmas-data-warehouse/>

- This repository is available as part of the AWS Open Data Program; therefore, egress fees are not charged to either the host or the person downloading the data
- These public S3 buckets are hosted by the CMAS Center on behalf of the U.S. EPA's Office of Research and Development, and the U.S. EPA's Office of Air and Radiation
- Metadata for the datasets in the CMAS Data Warehouse are available from the CMAS Dataverse site:

<https://dataverse.unc.edu/dataverse/cmascenter>

CMAS Data Warehouse

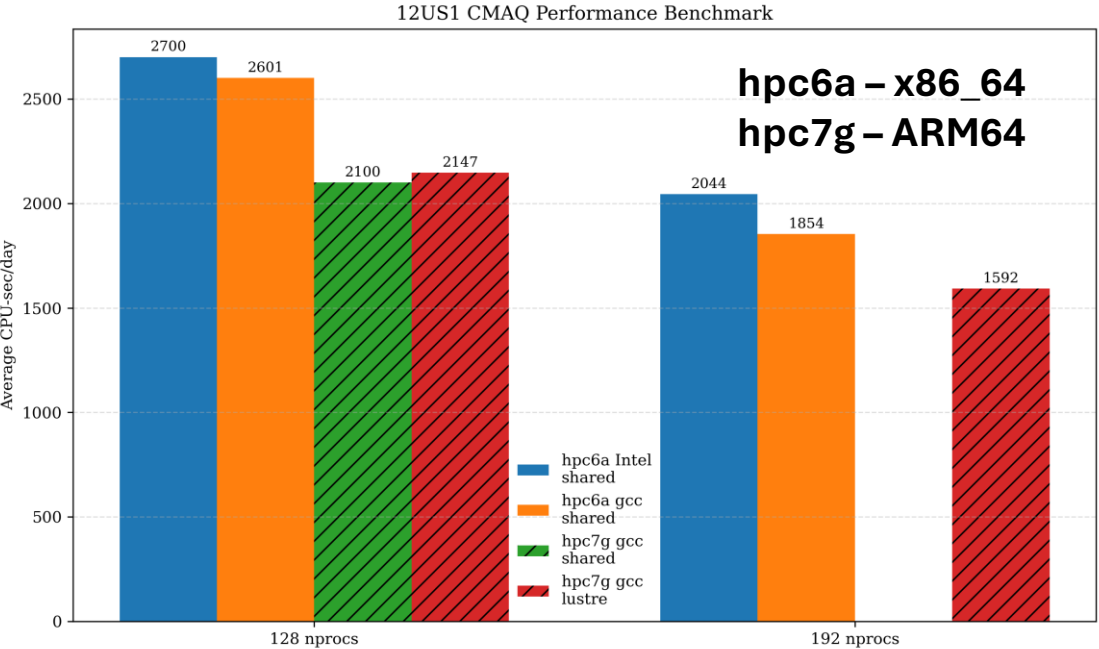


S3 Bucket	ncdump -k	Storage method	Extension	Size
CMAQ Input Data				
CMAQ Release Benchmark Data for Easy Download	tar.gz	archive	tar.gz	24.2 GiB
CMAQ CONUS-2 Benchmark Data	netcdf-3 classic	intact directory structure	.ncf	461.8 GiB
CMAQ Benchmark Data	netcdf-3 classic	intact directory structure	.nc	142.1 GiB (2018 12US1 data)
CMASWWLLN Lightning Data	netcdf-3 classic	intact directory structure	.ioapi	31.4 GiB
EQUATES EPA's Air QUALity Time Series Project Data	netcdf-4 compressed	intact directory structure	.ncf	4.3 TiB
CMAQ 2018 Modeling Platform	netcdf-4 compressed	intact directory structure	.nc4	6.1 TiB
AMET Observational Input Data				
AMET Data	netcdf-3 classic	intact directory structure	.nc	834.6 GiB
SMOKE Emissions Platforms Data				
2019 Modeling Platform	netcdf-3 classic	intact directory structure	ncf.gz	2.0 TiB
2016v3 Modeling Platform	netcdf-3 classic	mix	.camx/.ncf/zip	35.2 TiB
SMOKE 2016 Modeling Platform	netcdf-3 classic	mix	.ncf/zip	392.6 GiB

2023 36US3 Input data can be obtained from here : <https://zenodo.org/records/13737754>

Source : Simon, H et al., (2025). Expedited modeling of burn events results (EMBER): A screening-level dataset of 2023 ozone fire impacts in the US. *Data in Brief*, 58, 111208.

Benchmark Results (12US1)



- Increasing **nprocs** from **128** → **192** improves runtime for all configurations
- **hpc7g + Lustre** gives the best performance among the Graviton(ARM64) runs
- **Gcc on hpc6a (x86_64)** is faster against intel, though **hpc7g (ARM64) performs better for both 128 and 192 nprocs**
- Annual simulation runtime ranges from **~7–11 days for the 12US1 domain** depending on processor count and cluster configuration

Nodes	Instance Type	Cost (\$/hour)
2 nodes (128 nprocs)	hpc6a.48xlarge	\$5.91
2 nodes (128 nprocs)	hpc7g.16xlarge	\$3.44
3 nodes (192 nprocs)	hpc7g.16xlarge	\$5.12

Note: Here cost includes login node + compute nodes

The 12US1 benchmarks demonstrate good parallel scaling, where increasing processor counts improves runtime and the hpc7g + Lustre configuration provides the best performance among the tested ARM-based setups.

Key Findings

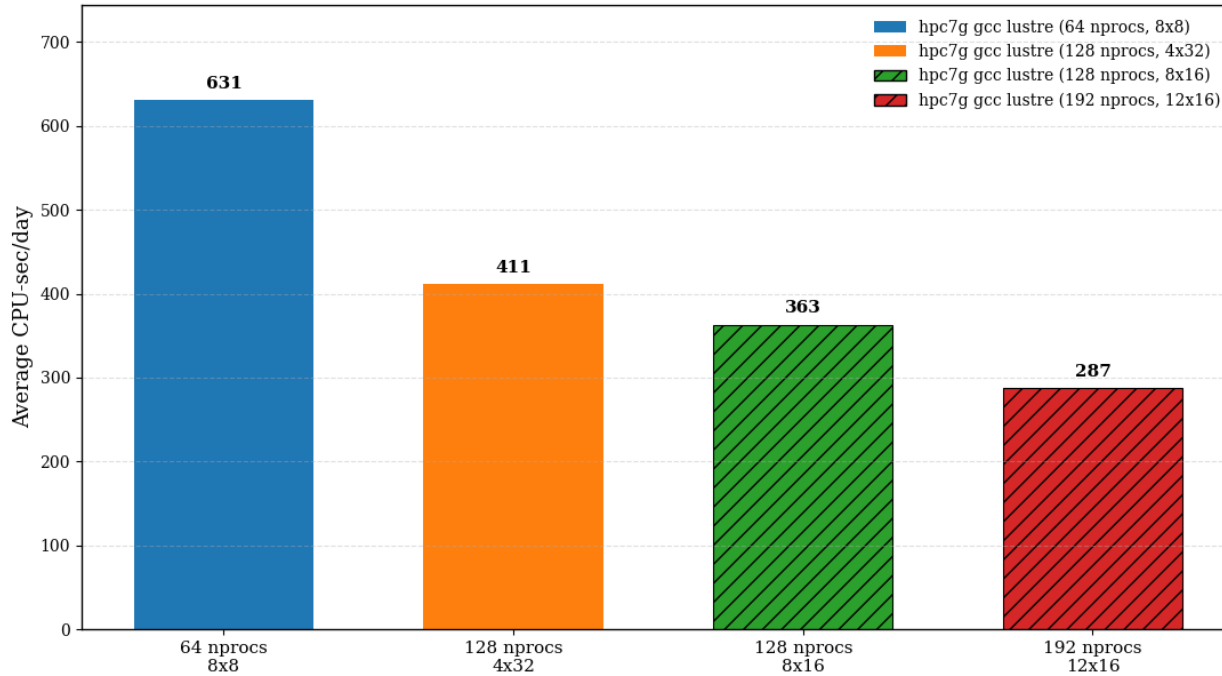


- **GCC outperformed** Intel compilers on x86_64 **by 4-10%** for 12US1
- GCC on ARM64 was **~24% faster than GCC** on x86_64 for 12US1
- Hpc7g (ARM64) instances offered **strong cost-performance**
- ARM processors reduce CMAQ compute cost by **~50% compared with x86_64 configurations**
- **ARM64 architecture** selected for **production runs for 36US3**
- FSx Lustre improved **parallel I/O performance**

Benchmark Results (36US3 on ARM64)



36US3 CMAQ Performance Benchmark



- Increasing **nprocs** from **64** → **192** **significantly** improves runtime
- 128 nprocs already provides **strong performance improvements** compared to **64**
- Best performance is **achieved with 192 nprocs** (3 nodes), reducing runtime from 3 to 1 day
- 36US3 domain covers a larger area but due to **coarse resolution**, runs are **much faster and cheaper than 12US1**
- Annual simulation runtime ranges **~1–3 days for the 36US3 domain**, depending on processor count and cluster configuration

Nodes	Instance Type	Cost (\$/hour)
2 nodes (128 nprocs)	hpc7g.16xlarge	\$3.44
3 nodes (192 nprocs)	hpc7g.16xlarge	\$5.12*

***Increasing the configuration from 2 nodes (\$3.44/hr) to 3 nodes (\$5.12/hr) increases compute cost by \$1.68/hr (~49%), while improving runtime by only ~26%.**

Storage Requirements



Domain	Daily Storage	Annual Storage
36US3	~7 GB/day	~3 TB
12US1	~90 GB/day	~36 TB

Note : Daily Storage includes inputs (meteorology, emissions , initial conditions, boundary Conditions) and outputs (2D and 3D)

FSx Lustre Storage Costs (Annual Run)



Domain	Provisioned Size	Cost
36US3	2,400 GB	~\$350
12US1	19,200 GB	~\$3,000

FSx for Lustre Storage for 12US1 (1 Month)

- Storage capacity: **36 TB × 1024 = 36,864 GB**
- Data compression (50%): **18,432 GB saved**
- Effective storage: **18,432 GB**
- Billed storage (rounded): 19,200 GB**

Cost Calculation (12US1)

- Price: **\$0.145 per GB-month**
- Storage cost: **19,200 × 0.145 ≈ \$3,000**
- Total monthly cost: ≈ \$3,000**

The cost estimate represents an annual CMAQ run, assuming the Lustre storage is provisioned for one month and includes cluster setup, benchmarking, simulation runtime, post-processing, and data transfer to Amazon S3 or local storage

Total Estimated Cost per Annual Run



- 12US1: ~\$800 –\$1,600 compute + ~\$3,000 storage
(cost range is based upon architecture, processor, domain decomposition and compiler used)
- 36US3: ~\$120 –\$220 compute + ~\$350 storage
- Storage corresponds to ~1 month Lustre usage
- Actual Lustre usage time typically shorter, based on user needs

Final Cost Summary

Domain	Compute Cost	Storage Cost	Total
12US1	\$800 – \$1,600	\$3,000	\$3,800 – \$4,600
36US3	\$120 – \$220	\$350	\$470 – \$570

Storage Strategy



- FSx for Lustre used during active simulations
- Provides high-performance parallel filesystem
- In our study, since we had multiple emissions scenarios that shared the same input data (meteorology, IC/BC), we created a shared drive. Once the simulation was completed, we copied onto shared and then post-processed and then archived to s3 bucket
- **Recommendation:**
 - **Store active simulation outputs in Amazon S3 Standard for fast access, while long-term archived data can be moved to S3 Glacier storage to significantly reduce storage costs (s3 costs in next slide)**

S3 bucket costing



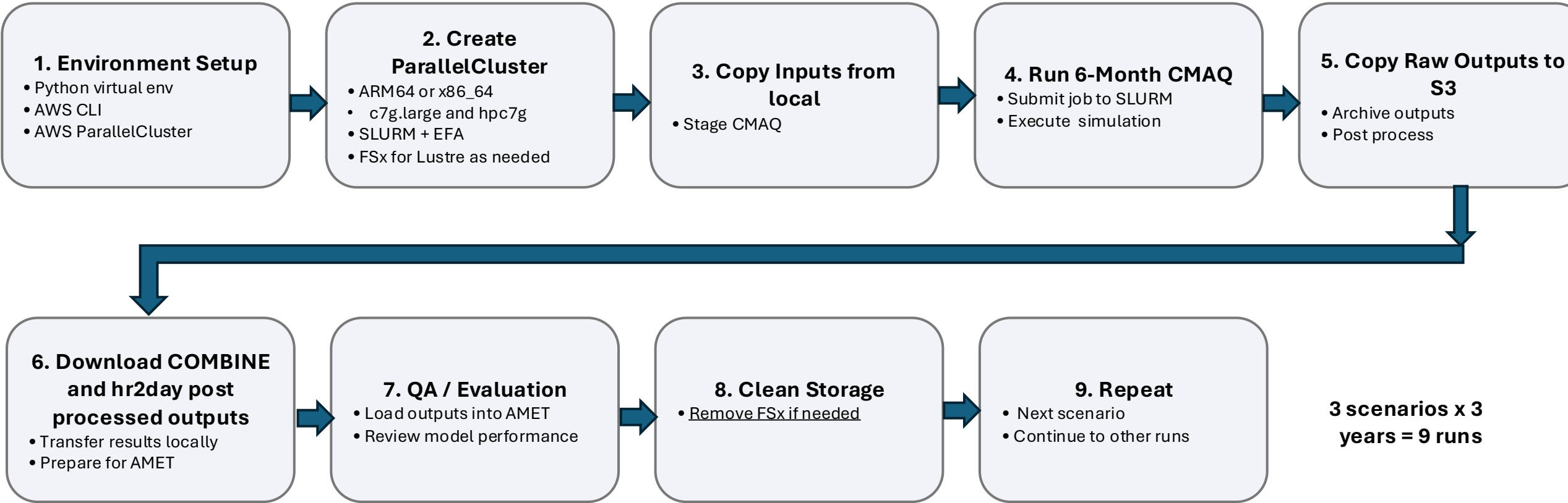
Storage Class	Typical Use Case	Retrieval Speed	Cost (USD / GB / Month)
S3 Standard	Frequently accessed simulation outputs and active analysis data	Milliseconds	\$0.023
S3 Standard – Infrequent Access	Data accessed occasionally but requiring fast retrieval	Milliseconds	\$0.0125
S3 Glacier Instant Retrieval	Archive data accessed occasionally (few times per year)	Milliseconds	\$0.004
S3 Glacier Flexible Retrieval	Long-term backups and archives	Minutes–Hours	\$0.0036
S3 Glacier Deep Archive	Very long-term archival (rarely accessed)	Up to 12 hours	\$0.00099

Using S3 Glacier Deep Archive can reduce storage cost by over 95% compared to S3 Standard for long-term archival data.

36US3 Study Workflow on AWS (hpc7g)



Study design: 6 months simulated (April–September) for 3 years, each with 3 emissions scenarios | Total = 9 CMAQ runs



Lesson Learned (How to save costs)



- **Estimated costs ~2x lower** (~\$2,000 vs ~\$4,000 actual), as earlier costs increased due to CMAQ version changes, repeated runs, and no Lustre compression
- **Storage costs reduced** using compressed, cost-efficient Lustre ($\approx 4x$ cheaper than 50 MBps/TiB) with **Persistent (125 MBps/TiB)** or **Scratch (200 MBps/TiB)** throughput
- Use **small root and /shared volumes**, keep all **I/O on Lustre**, and **disable Lustre when not in use** to save costs
- **Cost calculator example** shown for **Persistent Lustre** with **50 and 125 MBps/TiB** configurations

FSx for Lustre Storage Cost (Monthly)

Storage capacity: $3 \text{ TB} \times 1024 = 3,072 \text{ GB}$

Data compression saving (50%): $3,072 \times 0.5 = 1,536 \text{ GB saved}$

Effective storage: $3,072 - 1,536 = 1,536 \text{ GB}$

Billed Storage : 2400 GB (either 1.2 TB or chunks of 2.4 TB)

50 Mbps/TiB

Price: **\$0.60 per GB-month**

Storage cost: $2,400 \text{ GB} \times \$0.60 = \sim \$1500$

125 Mbps/TiB

Price: **\$0.145 per GB-month**

Storage cost: $2,400 \text{ GB} \times \$0.145 = \sim \$350$

Cost and Performance Advantages of ARM64 (Graviton 3E)



- Better price to performance ratio
 - ARM64 was **24% faster than x86_64** in CMAQ 12US1 benchmarking using the **gcc compiler**
- Lower compute and login node cost
 - Over **50% savings for login nodes** and **40% savings for compute nodes** compared to Intel x86_64 instances
- Improved Efficiency for CMAQ
 - Provides faster simulations with **lower overall cloud computing costs**

Recommended Configuration



- Compute: hpc7g instances (Also depends upon your application)
- Compiler: GCC
- Storage: FSx for Lustre
- Delete Lustre after simulation
 - move raw CMAQ outputs to s3 glacial

Advantages of AWS ParallelCluster



- Scalable HPC environment
- Automated cluster management
- Integration with AWS storage services
- Suitable for research workflows

Implications for CMAQ Community



- Cloud HPC enables flexible research infrastructure
- ARM processors reduce simulation cost
- Optimized storage strategies minimize expenses
- Useful for multiple long-term simulations

Future Work



- Benchmark CMAQ-DDM with multiple sensitivity variables
- Evaluate additional new compute instances and storage options
 - As AWS releases new compute nodes (e.g., hpc8a)
 - As EPA releases new versions of CMAQ
- Automate CMAQ workflows in cloud
 - Provisioning compute nodes, pull input data from s3bucket, submitting jobs, post processing, archive outputs to to s3 bucket or local drive, removal of resources after job completion
- Improve cost optimization strategies
 - Efficient storage options, choosing right size compute resources, use HPC instances, auto scaling and shut down idle resources, optimize data transfer (compression), cost allocation tags

References



- CMAQ Parallel Cluster Tutorial
 - <https://pcluster-cmaq.readthedocs.io/en/latest/>
 - <https://github.com/CMASCenter/pcluster-cmaq>
- CMAQ on AWS workshop
 - <https://catalog.workshops.aws/cmaq-tutorial/en-US/>
- Efstathiou et al., (2024). Enabling high-performance cloud computing for the Community Multiscale Air Quality Model (CMAQ) version 5.3. 3: performance evaluation and benefits for the user community. *Geoscientific model development*, 17(18), 7001-7027.
- CMAQ Documentation
 - <https://github.com/USEPA/CMAQ>
- AWS ParallelCluster Documentation
 - <https://github.com/aws/aws-parallelcluster>
- AWS FSx for Lustre Pricing
 - <https://aws.amazon.com/fsx/lustre/pricing/>

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- The U.S. EPA CMAQ Development Team

Disclaimer : The views expressed here are those of the authors and do not necessarily reflect the views and policies of the US Environmental Protection Agency (EPA) or Cloud Service Provider (Amazon).

Questions



- Thank you
- Questions?

Additional Slides



Instructions to add and remove lustre drive



Updating the CMAQ Cluster

1. Stop the compute fleet before updating the cluster

```
pcluster update-compute-fleet --cluster-name cmaq --status STOP_REQUESTED
```

2. Update the cluster configuration to add FSx for Lustre storage

```
pcluster update-cluster -n cmaq -c hpc7g.16xlarge.fsx.yaml
```

3. Check the compute fleet status

```
pcluster describe-compute-fleet --cluster-name cmaq
```

Proceed once the status indicates the update is complete.

4. After the simulation and data transfer are complete, remove the FSx for Lustre storage

```
pcluster update-cluster -n cmaq -c hpc7g.16xlarge.nofsx.yaml
```

5. Restart the compute fleet after the cluster update

```
pcluster update-compute-fleet --cluster-name cmaq --status START_REQUESTED
```

Example hpc7g.16xlarge.fsx.yaml file



```
Region: us-east-1
Image:
  Os: ubuntu2204
HeadNode:
  InstanceType: c7g.large
Networking:
  SubnetId: subnet-07e412a0ca36ad7fa
DisableSimultaneousMultithreading: true
Ssh:
  KeyName: ubuntu
LocalStorage:
  RootVolume:
    Size: 200
    Encrypted: false
    VolumeType: gp3
    DeleteOnTermination: false
Scheduling:
  Scheduler: slurm
  SlurmSettings:
    ScaledownIdleTime: 3
  SlurmQueues:
    - Name: queue1
      CapacityType: ONDEMAND
      Networking:
        SubnetIds:
          - subnet-07e412a0ca36ad7fa
      PlacementGroup:
        Enabled: true
```

```
ComputeResources:
  - Name: compute-resource-1
    InstanceType: hpc7g.16xlarge
    MinCount: 0
    MaxCount: 12
    DisableSimultaneousMultithreading: true
    Efa:
      Enabled: true
      GdrSupport: false
SharedStorage:
  - MountDir: /shared
    Name: ebs-shared
    StorageType: Ebs
    EbsSettings:
      Encrypted: false
      Size: 1200
  - MountDir: /fsx
    Name: name2
    StorageType: FsxLustre
    FsxLustreSettings:
      StorageCapacity: 1200
  ~
```

Delete this and save it as other yaml with the steps from previous slide save it with nofsx tag

Settings for compression and choosing persistent drive 2 to save cost



- SharedStorage:
 - Name: FsxLustre0
 - StorageType: FsxLustre
 - MountDir: /fsx
 - FsxLustreSettings:
 - DeletionPolicy: Retain
 - StorageCapacity: 1200
 - DeploymentType: PERSISTENT_2
 - PerUnitStorageThroughput: 125
 - DataCompressionType: LZ4