

AWS re:Invent

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CMP305

Best practices for high performance computing in the cloud

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Agenda

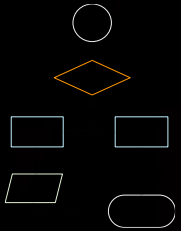
Presentation: Fundamentals of infrastructure for HPC and AWS ParallelCluster

Hands-on: Create a HPC cluster using AWS ParallelCluster

Presentation: Amazon FSx for Lustre and application management using Spack

Hands-on: HPC cluster update to dynamically mount Amazon FSx for Lustre

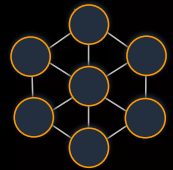
Compute and orchestration building blocks



Workflow, notifications, queues

- Workflow management
- Notification and message queues

Workflow management and communication

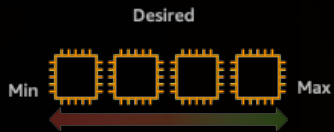


Serverless & containers

- Event-driven functions (AWS Lambda)
- Batch schedulers; containers orchestrators

Abstraction

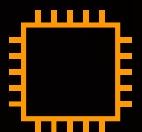
Focus on the workload and not infrastructure



Provisioning

- Amazon EC2 Auto Scaling groups: scale up & down
- Instance fleets: capacity at scale across AZs

Compute on events or requests



Instances

- Virtualized
 - Bare metal
- } Different capabilities (CPU, RAM, SSD, network, and accelerators)

Base compute layer

Base infrastructure

VPC and subnets

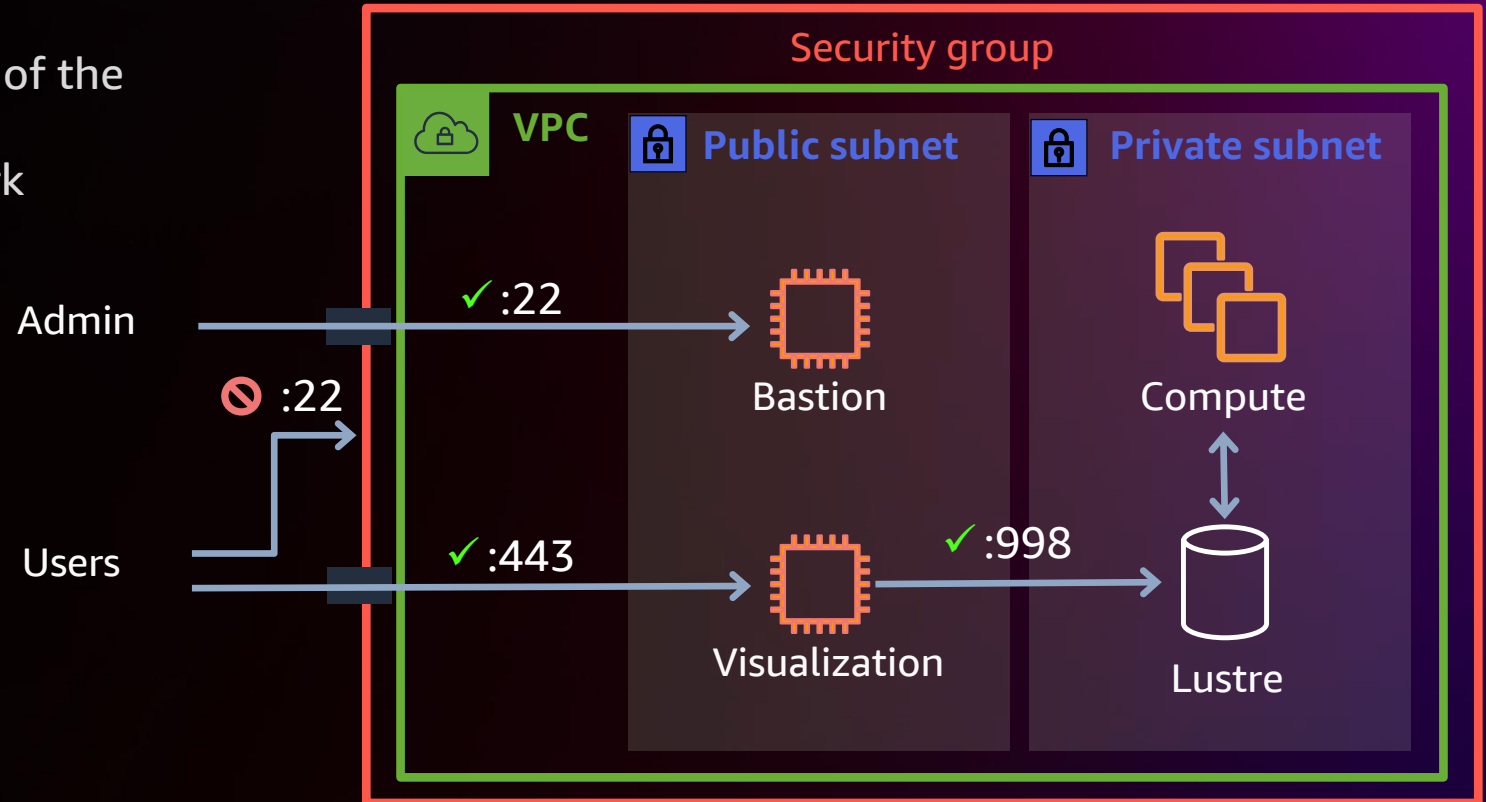
- Virtual private cloud: logical section of the cloud provider infrastructure
- Subnet: logical partition of a network

Security groups

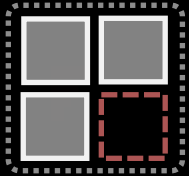
- Virtual firewalls
- VPC & instances

Instances and services

- Instances
- Managed services
- ...

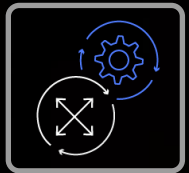


Amazon EC2 Auto Scaling in more detail



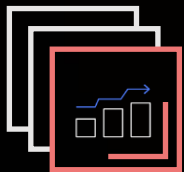
Logical unit

Purpose of scaling or management



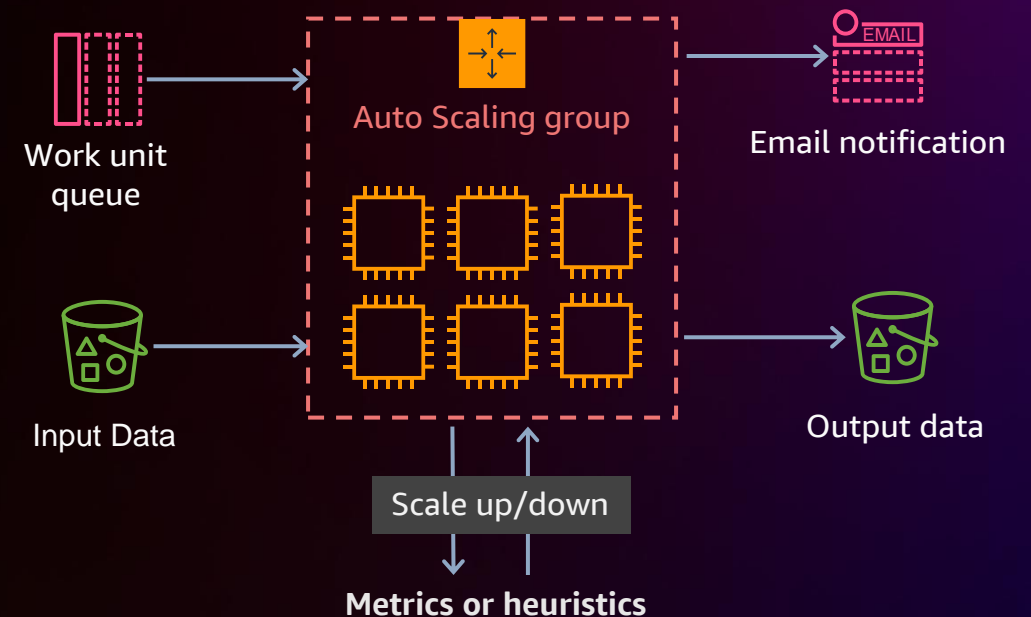
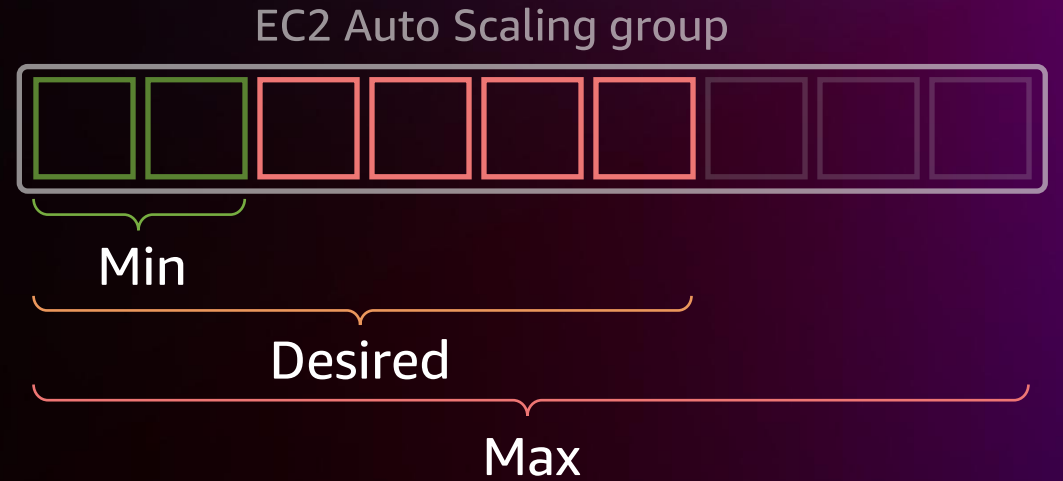
Launch templates

Kind, size, storage, SSH key pair, user data, and security groups



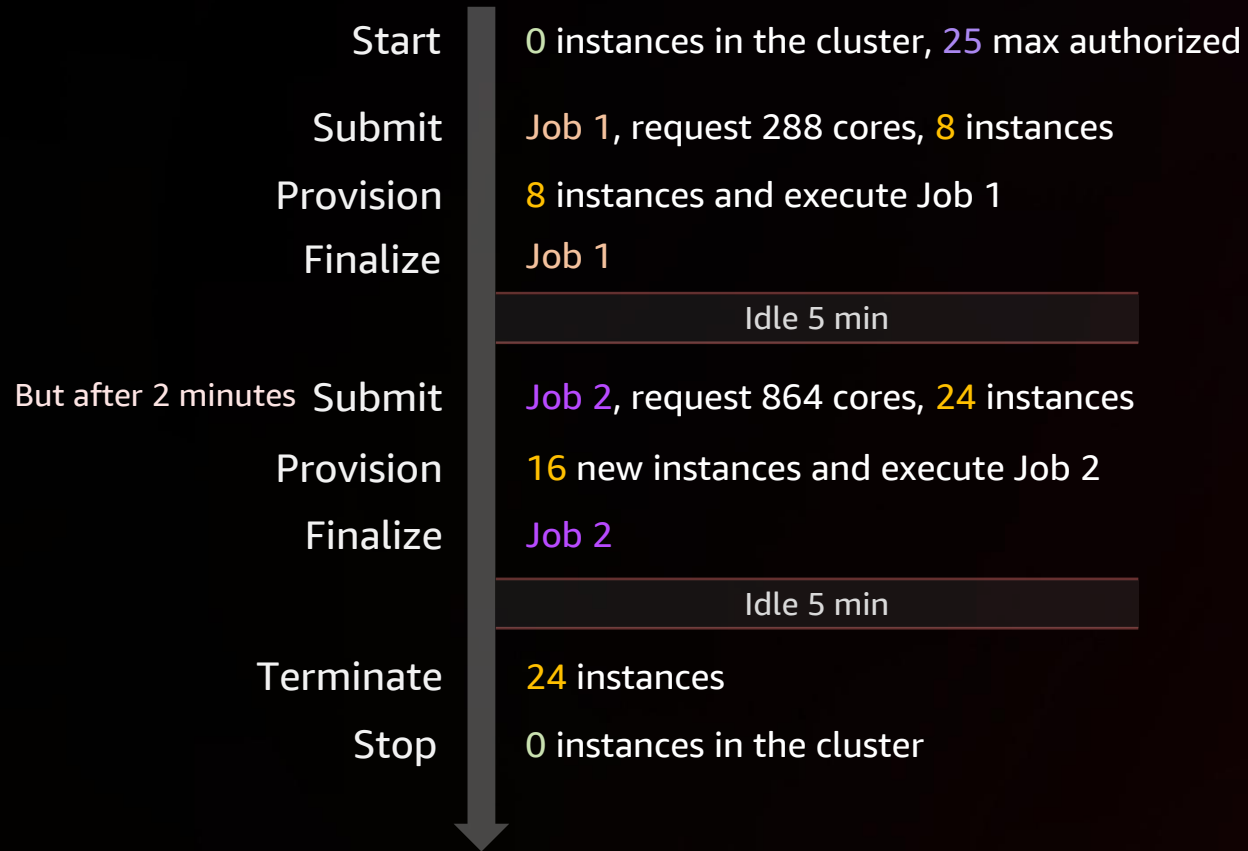
Scaling options

- Manual, schedule, predictive
- Notify on start, stop, terminate . . .



EC2 Auto Scaling compute system?

Imagine that nodes are added when jobs are submitted and removed when they finish



Auto Scaling compute cluster



Min: 0 Desired: 24 Max: 25
cores / node: 36

```
aws autoscaling delete-scaling-group \
--auto-scaling-group-name my-asg-scaling-group \
--desired-capacity 0 \
--launch-template my-launch-template \
--image-id ami-0c6426461090 \
--min-size 1 --max-size 25 \
--vpc-subnet-ids vpc-1a2b3c4d subnet-5ea0c127
```

Putting it all together

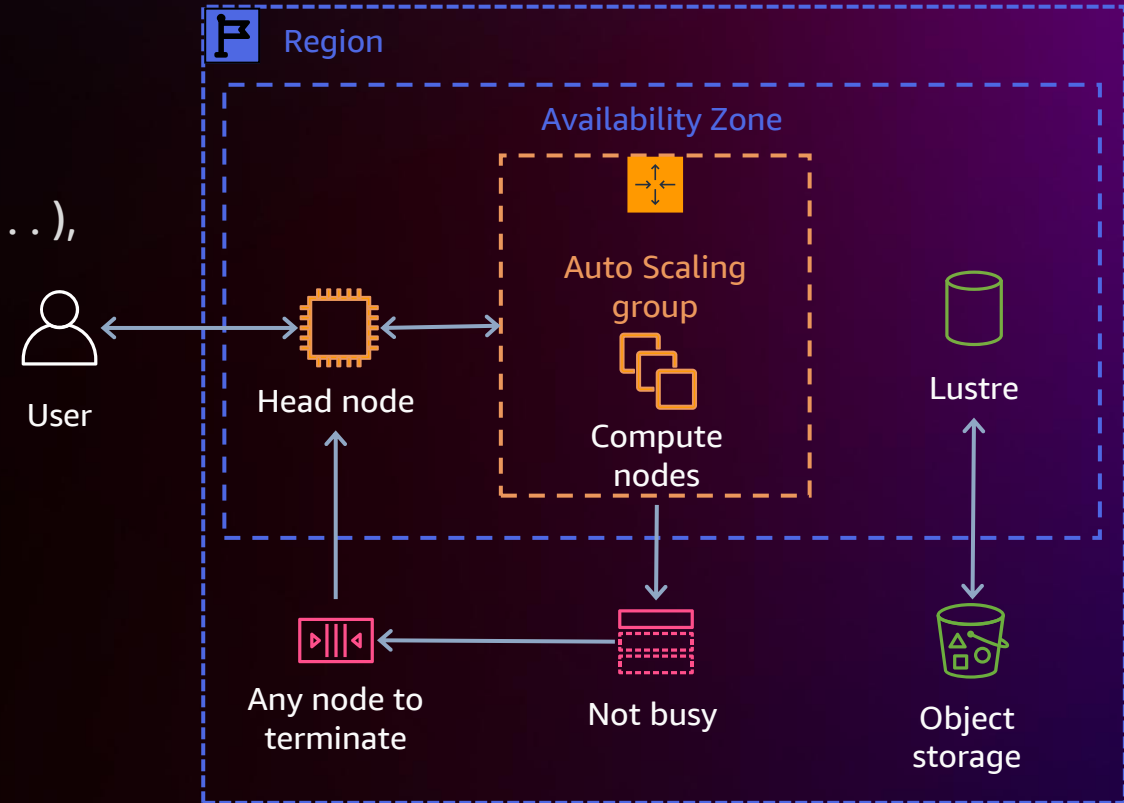
Building an auto-scaling HPC cluster

- Similar to on premises but with auto scaling
- Still a classical HPC system with a scheduler (SLURM, SGE, . . .), Lustre, and placement groups (tightly coupled)
- The same familiar interface with an elastic capacity

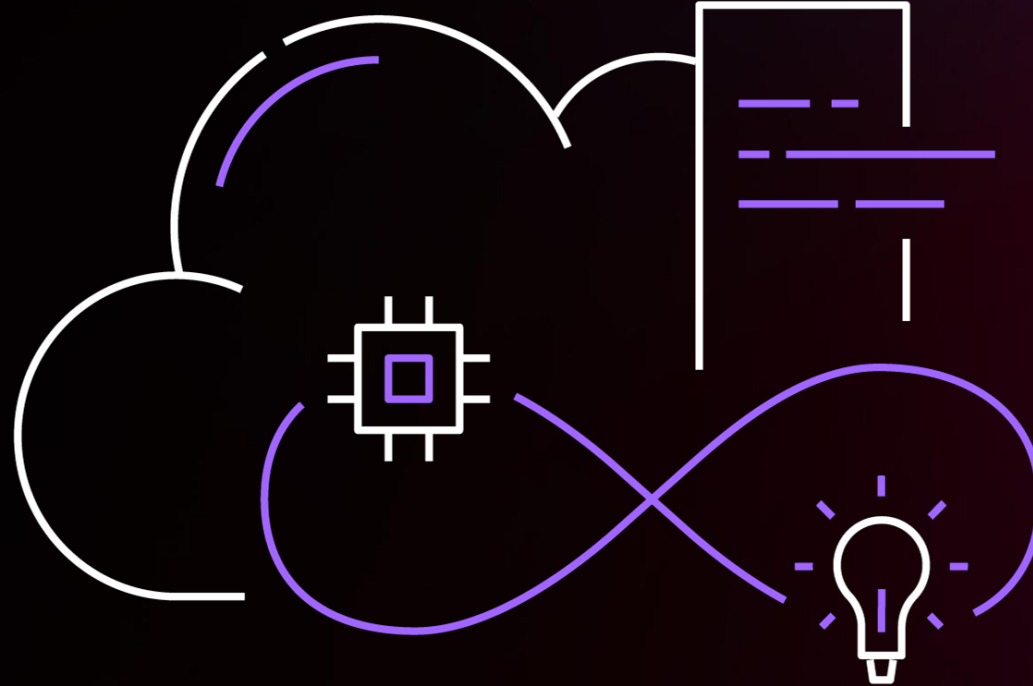
Additional technical considerations

When ready, instances send notifications to a message queuing service – the scheduler watches this queue and adds the compute nodes as they appear

When not busy, they will lock themselves up, check the scheduler queue, send a notification, and terminate



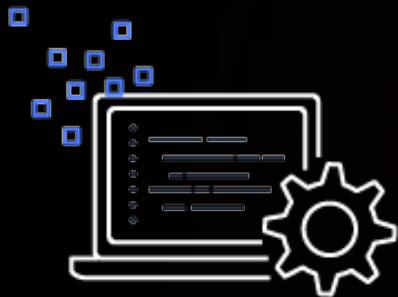
Part of the next hands-on



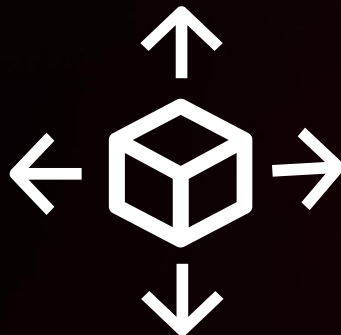
AWS ParallelCluster

Open-source cluster management for HPC on AWS

Why use AWS ParallelCluster?



Easy cluster management



Automatic resource scaling



Seamless migration to the cloud

Easy cluster management



“pcluster configure” to set up
a cluster in minutes

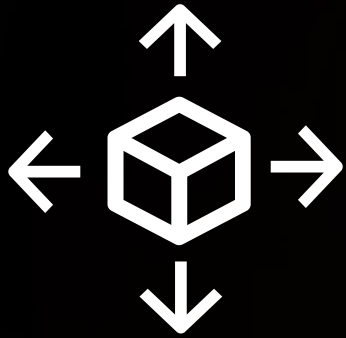


Use config files to define
details of replicable clusters

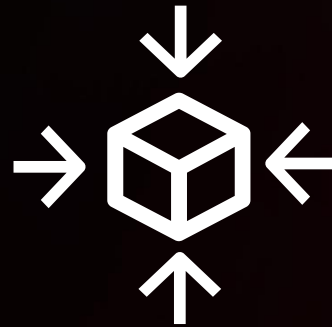


Launch, stop, and restart clusters
on demand

Automatic resource scaling



Scale up when jobs
are waiting

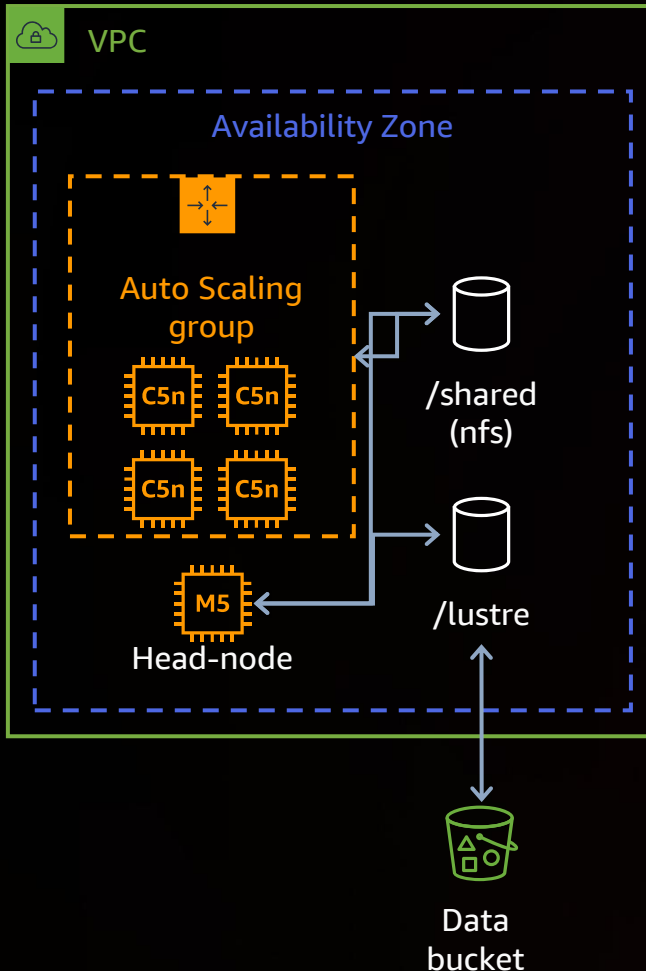


Scale down when the
cluster is idle



Your data storage and file system
scale to match your compute

Simple architecture



- Post install configuration
 - Install applications scripts
- Amazon EBS snapshot bootstrap
 - Application installations or static configurations
- Other details
 - Amazon EFS can be shared across clusters
 - Lustre partition can be mounted but per AZ
 - Public/private subnets for head/compute
 - Link to AD for user mapping if required

Example of configuration file

Region: [AWS_REGION]

Image:

Os: alinux2

SharedStorage:

- Name: Ebs0

StorageType: Ebs

MountDir: /shared

EbsSettings:

VolumeType: gp3

DeletionPolicy: Delete

Size: '100'

HeadNode:

InstanceType: c5.xlarge

Ssh:

KeyName: [KEY_NAME]

Networking:

SubnetId: [subnet-12345689]

Dcv:

Enabled: true

LocalStorage:

RootVolume:

VolumeType: gp2

Scheduling:

Scheduler: slurm

SlurmQueues:

- **Name:** compute-queue

ComputeResources:

- Name: hpc6a

MinCount: 0

MaxCount: 4

InstanceType: hpc6a.48xlarge

Efa:

Enabled: true

DisableSimultaneousMultithreading: true

Networking:

SubnetIds:

- [subnet-12345689]

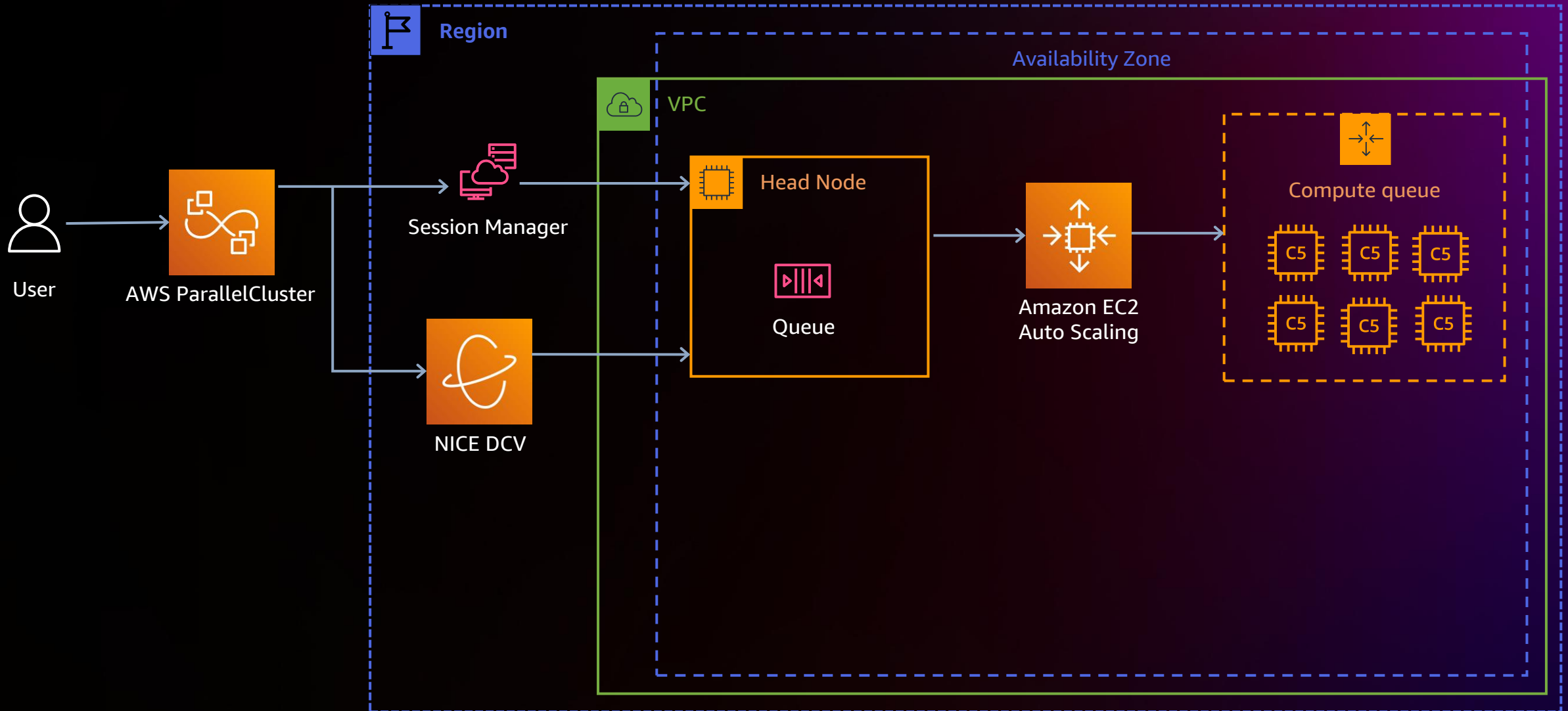
PlacementGroup:

Enabled: true



Hands-on: Create a HPC cluster using AWS ParallelCluster

Architecture for this workshop



Getting started with this workshop

- As a participant, you will have access to an AWS account with any optional pre-provisioned infrastructure and IAM policies needed to complete this workshop
- The AWS account will only be available for the duration of this workshop; you will lose access to the account thereafter
- The optional pre-provisioned infrastructure will be deployed to a specific region; check your workshop content to determine whether other regions will be used
- Be sure to review the terms and conditions of the event; do not upload any personal or confidential information in the account

Step 1: Sign-in via your preferred method

<https://catalog.workshops.aws/join>



aws workshop studio

Workshop Studio > Sign in

Sign in

Choose a preferred sign-in method

Email one-time password (OTP)

Enter your personal or corporate email to receive a one-time password

Login with Amazon

Login with your Amazon.com retail account

Amazon employee

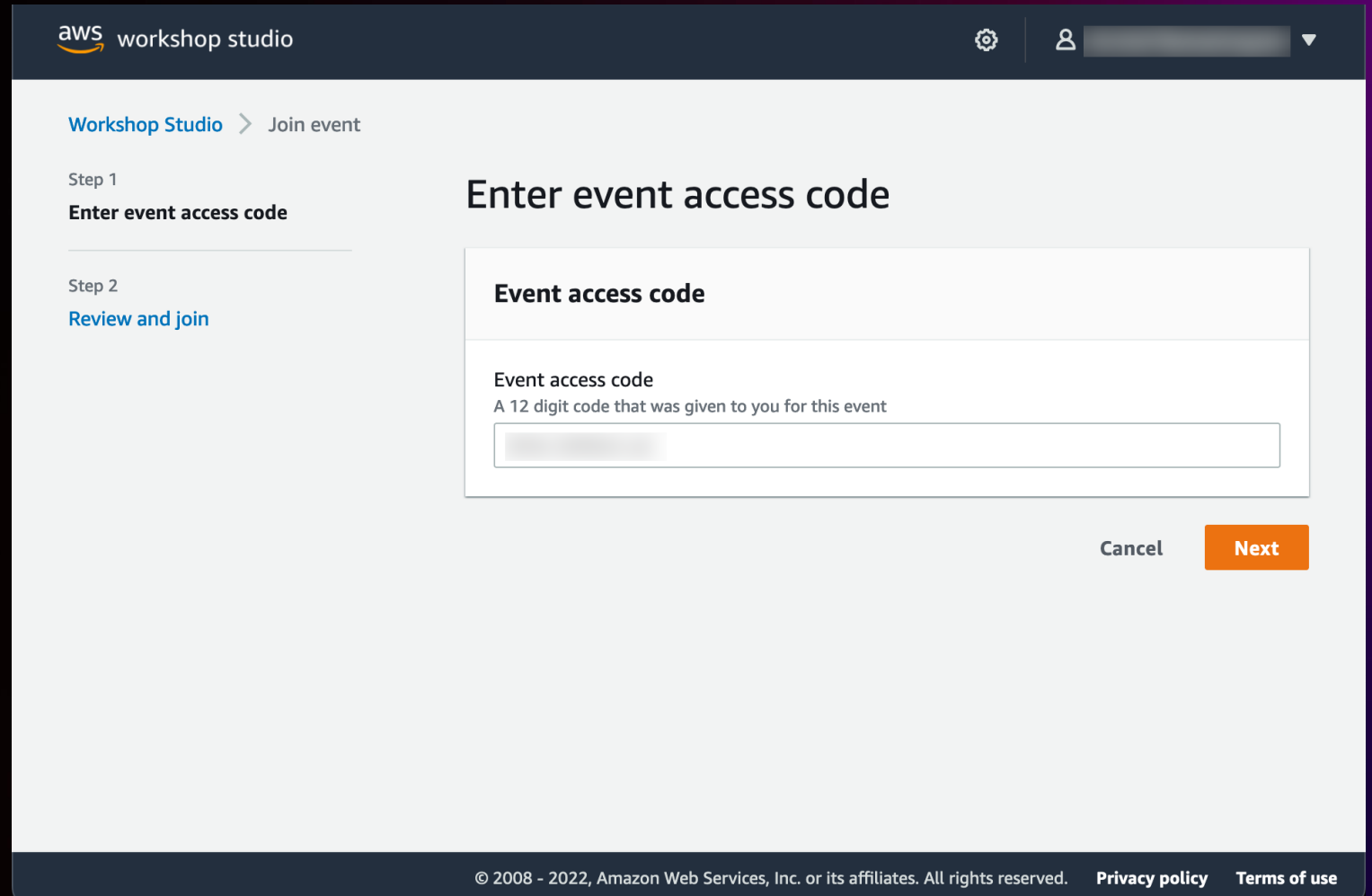
Login with your Amazon Corporate account. Only for Amazon Employees.

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Step 2: Enter event access code

Enter 12-digit event access code

If you were given a one-click join link, you can skip this step



The screenshot shows the AWS Workshop Studio interface for joining an event. The top navigation bar includes the AWS logo, 'workshop studio', a settings gear icon, a user profile icon, and a dropdown arrow. Below the navigation bar, the breadcrumb 'Workshop Studio > Join event' is displayed. The main content area is titled 'Enter event access code'. On the left, a progress indicator shows 'Step 1: Enter event access code' as the current step and 'Step 2: Review and join' as the next step. The main form area has a title 'Event access code' and a description: 'Event access code' followed by 'A 12 digit code that was given to you for this event'. Below this is a text input field. At the bottom right of the form area are two buttons: 'Cancel' and 'Next'. The footer contains the copyright notice '© 2008 - 2022, Amazon Web Services, Inc. or its affiliates. All rights reserved.' and links for 'Privacy policy' and 'Terms of use'.

aws workshop studio

Workshop Studio > Join event

Step 1
Enter event access code

Step 2
Review and join

Enter event access code

Event access code




Event access code
A 12 digit code that was given to you for this event

Cancel Next

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Step 3: Review terms and join event

aws workshop studio

Workshop Studio > Join event

Step 1
[Enter event access code](#)

Step 2
Review and join

Review and join

Event details

Name	Start time	Duration	Level
AWS General Immersion Day	9/23/2022 01:13 AM	12 hours	-

Description
AWS General Immersion Day

Terms and Conditions

Read and accept before joining the event

1. By using AWS Workshop Studio for the relevant event, you agree to the AWS Event Terms and Conditions and the AWS Acceptable Use Policy. You acknowledge and agree that are using an AWS-owned account that you can only access for the duration of the relevant event. If you find residual resources or materials in the AWS-owned account, you will make us aware and cease use of the account. AWS reserves the right to terminate the account and delete the contents at any time.
2. You will not: (a) process or run any operation on any data other than test data sets or lab-approved materials by AWS, and (b) copy, import, export or otherwise create derivate works of materials provided by AWS, including but not limited to, data sets.
3. AWS is under no obligation to enable the transmission of your materials through Event Engine and may, in its discretion, edit, block, refuse to post, or remove your materials at any time.
4. Your use of AWS Workshop Studio will comply with these terms and all applicable laws, and your access to AWS Workshop Studio will immediately and automatically terminate if you do not comply with any of these terms or conditions.

☒ I agree with the Terms and Conditions

Cancel

Previous

Join event

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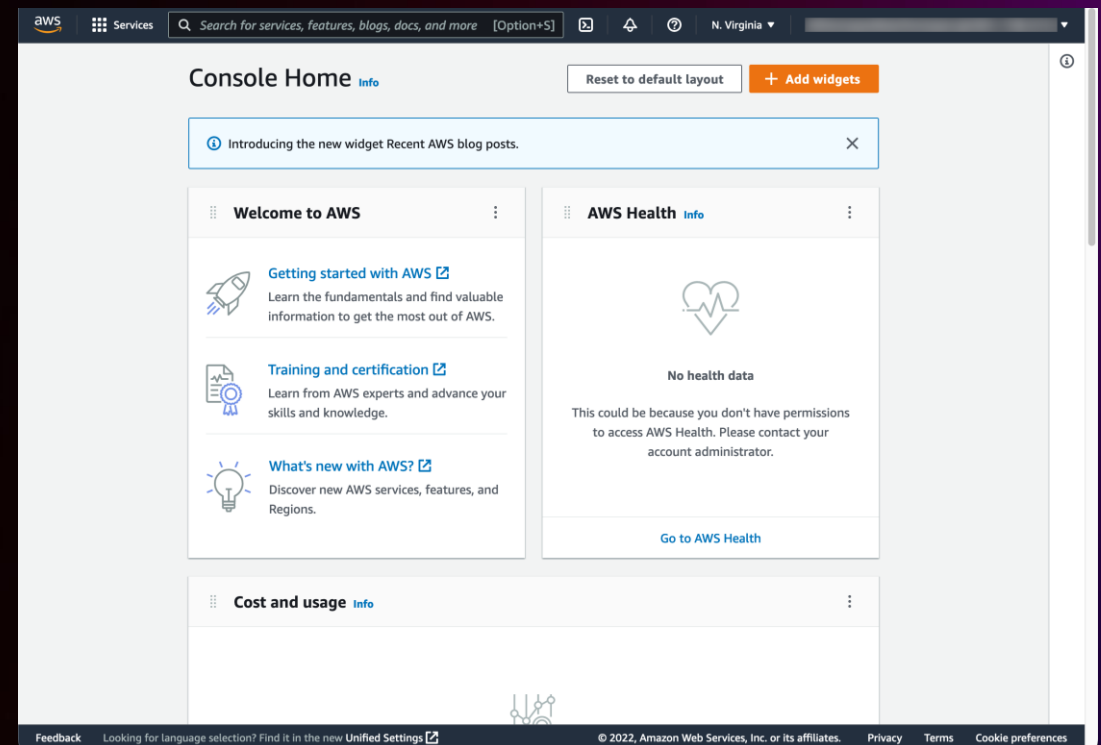
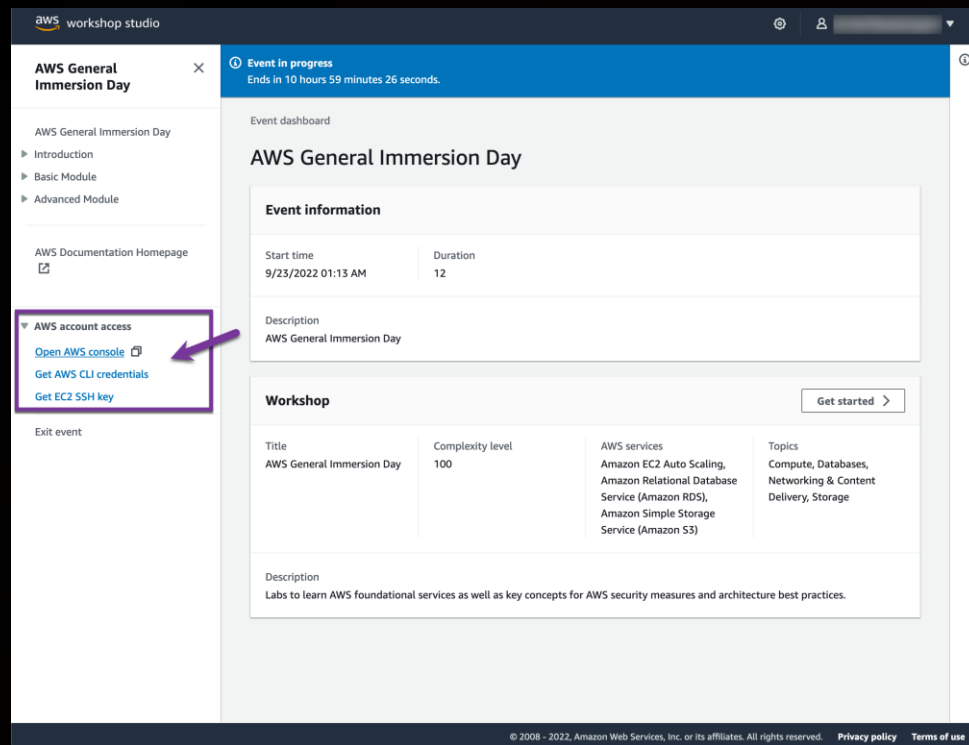
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Step 4: Access AWS account

Access the AWS Management Console or generate AWS CLI credentials as needed



Step 5: Get started with the workshop

The screenshot shows the 'Event dashboard' for the 'AWS General Immersion Day' workshop. The left sidebar contains navigation links: 'AWS General Immersion Day' (with sub-links for Introduction, Basic Module, and Advanced Module), 'AWS Documentation Homepage', 'AWS account access' (with links for 'Open AWS console', 'Get AWS CLI credentials', and 'Get EC2 SSH key'), and 'Exit event'. The main content area displays 'Event information' (Start time: 9/23/2022 01:13 AM, Duration: 12) and 'Workshop' details (Title: AWS General Immersion Day, Complexity level: 100, AWS services: Amazon EC2 Auto Scaling, Amazon Relational Database Service (Amazon RDS), Amazon Simple Storage Service (Amazon S3), Topics: Compute, Databases, Networking & Content Delivery, Storage). A 'Get started' button with a right-pointing arrow is located at the bottom right of the workshop details section, highlighted by a purple arrow.



The screenshot shows the 'Workshop' page for the 'AWS General Immersion Day' workshop. The left sidebar is identical to the previous screenshot. The main content area features the 'IMMERSION DAYS' logo, which is a stylized brown helmet with a white visor. Below the logo, the text reads: 'In this General Immersion Day workshop, through a mix of service explanation and hands-on labs led by AWS, you will learn about AWS foundational services as well as key concepts for AWS security measures and architecture best practices. The hands-on labs are largely divided into **basic and advanced modules**. In basic modules, you can learn various features of each AWS foundational service. In advanced modules, you can learn how to connect each service organically to create architecture like 3-tier web application.' At the bottom right, there are 'Previous' and 'Next' buttons.

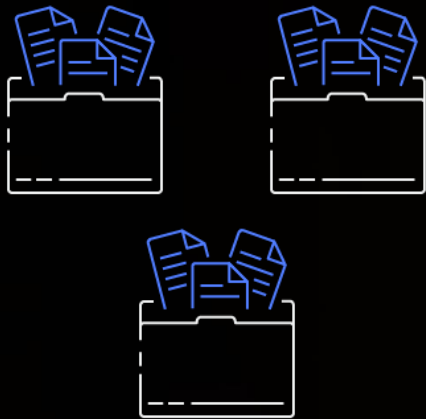
Amazon FSx for Lustre



Storage should not be the bottleneck for compute-intensive workloads

Faster storage reduces time to results and overall TCO by saving compute costs

Vast datasets

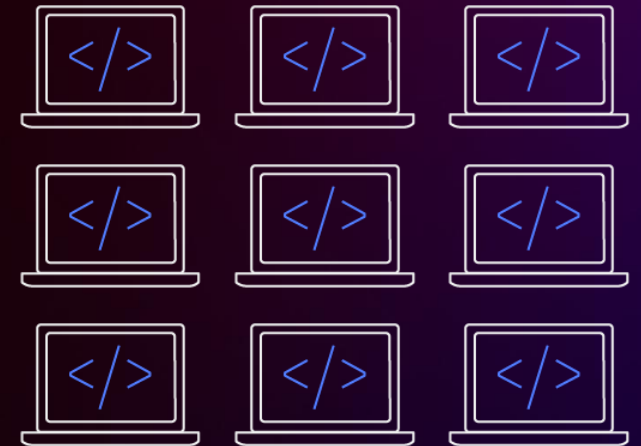


Ability to serve data quickly:

Fast storage
High-speed network
Low latency



Scale out compute capacity
(hundreds to millions of cores)



Amazon FSx for Lustre



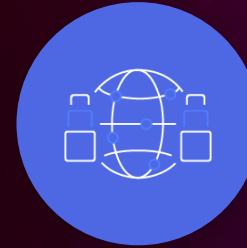
Fully managed Lustre file system for high-performance workloads



Massively scalable
performance



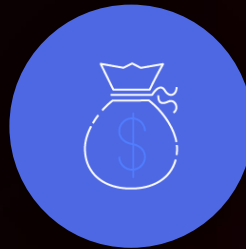
Seamless access to
your data repositories



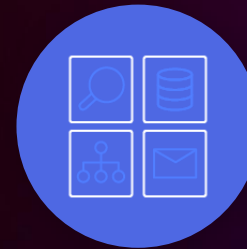
Simple and
fully managed



Native file
system interface



Cost optimized for
compute-intensive workloads



Secure
and compliant

High, scalable performance



High, scalable
performance

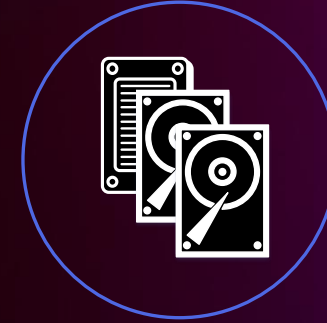
SSD



Scratch

Short-term processing
Spin up → process → spin down
Single copy of data

SSD or HDD



Persistent

Longer-term processing
Highly available (HA) file servers
Replicated copies of data

Amazon FSx for Lustre control plane (API, management layer, file system control) is designed to be HA for both options

What FSx for Lustre brings to your workloads

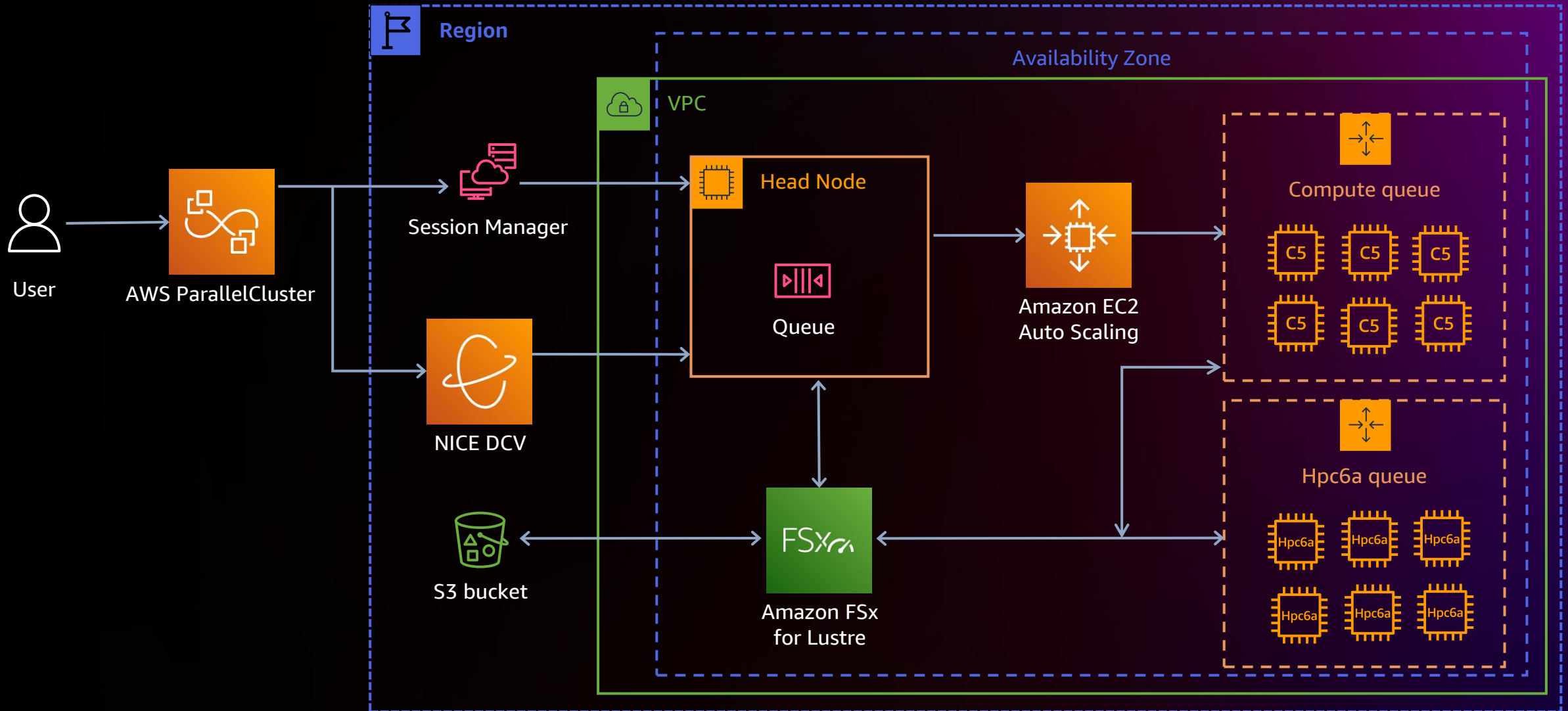


**Access to Amazon S3
data** through a fast
file interface



Hands-on: HPC cluster update to use Amazon FSx for Lustre

Architecture for this workshop



Thank you!

Maxime Hugues
maxhaws@amazon.com

Lowell Wofford



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survey in the **mobile app**



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