AWS re:Invent

NOV. 29 – DEC. 3, 2021 | LAS VEGAS, NV

CMP405

The future of computational fluid dynamics in the cloud

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Agenda

Introduction

What is CFD, and why does it matter?

1. Compute selection

2. Storage

3. Visualization

4. Cost optimization

5. Innovating with ML

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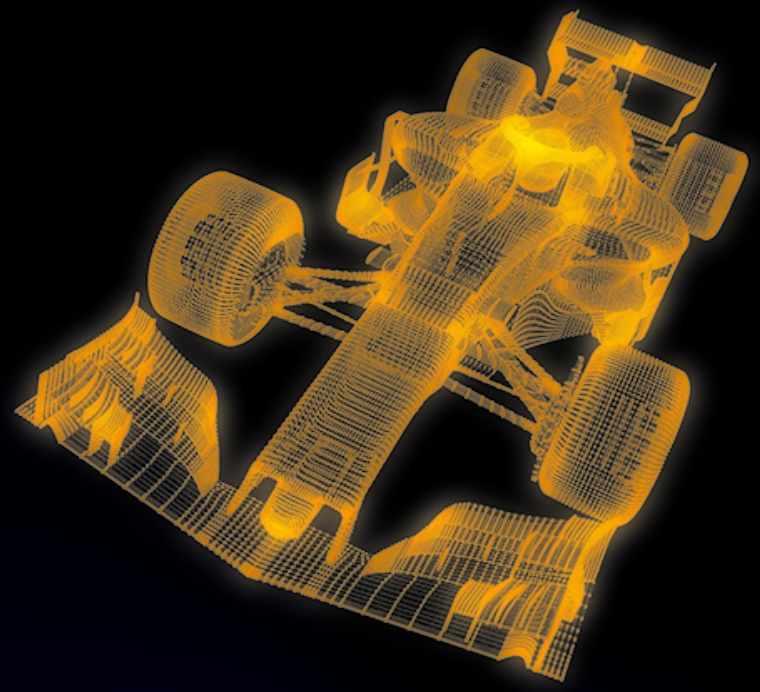
What is CFD, and why does it matter?

Companies need a way to assess the performance of new designs

The common goal is to go from conceptual design to full design in the shortest possible time with the least expense

Physical tests are difficult; specifically, they are expensive and time-consuming



Formula 1 on AWS

Formula 1 designed the 2022 car using CFD models on AWS – they faced several challenges with traditional methods

- **No access to wind tunnels** for 12 to 24 months, only CFD
- **60 hours** to **10 hours** thanks to AWS

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Agility = the right tool for the job

Company	Simulator(s)	Hardware
Ansys	Fluent	CPU, GPU
Dassault	Abaqus	CPU, GPU
Siemens	Star-CCM+	CPU
LSTC/Ansys	LS-DYNA	CPU, GPU
OpenFOAM Foundation	OpenFOAM	CPU, GPU
Comsol	Multiphysics	CPU
Altair	AcuSolve	CPU

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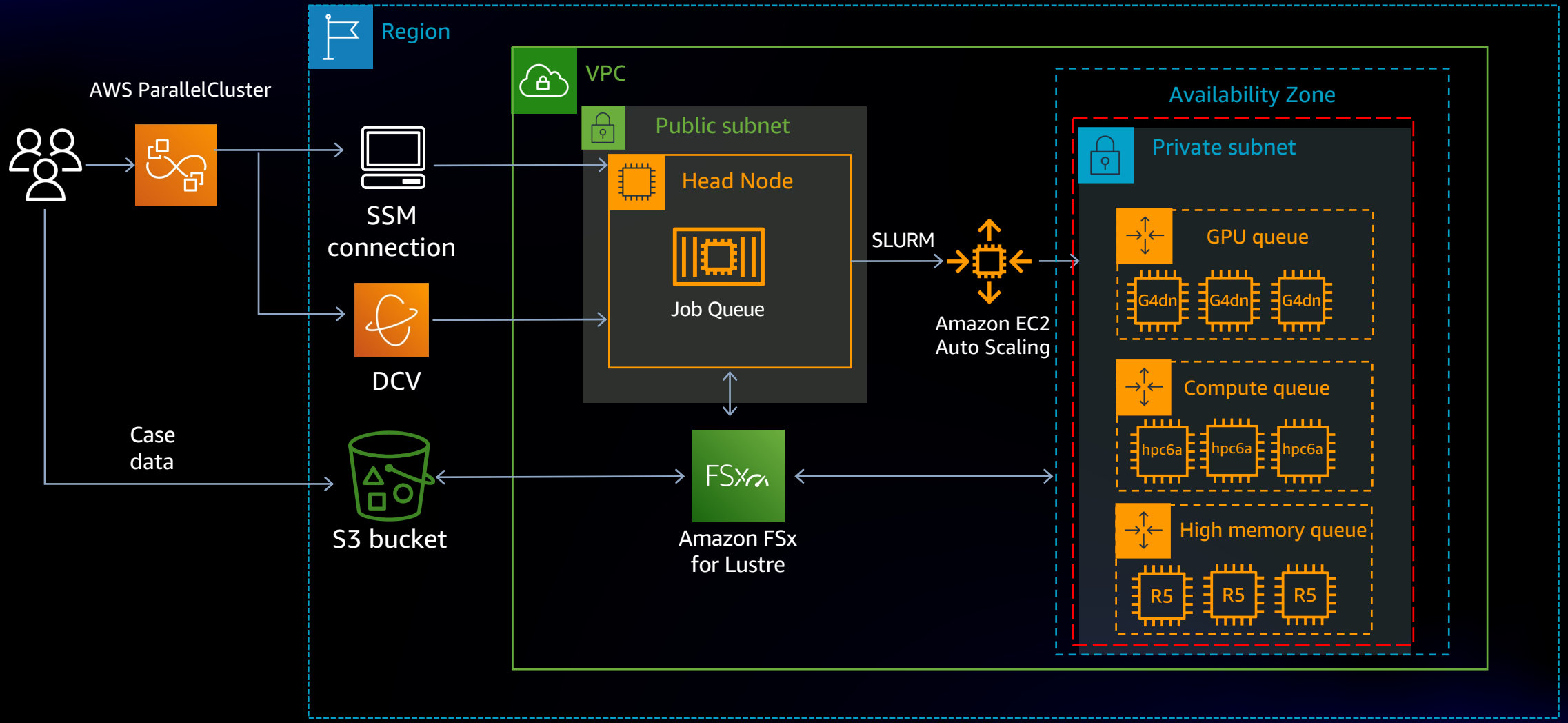
Reference architecture



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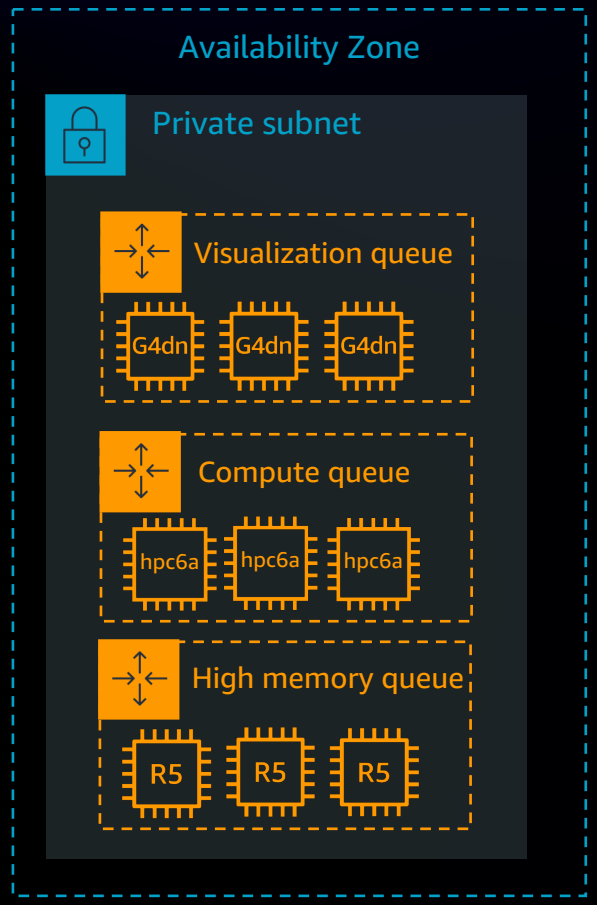
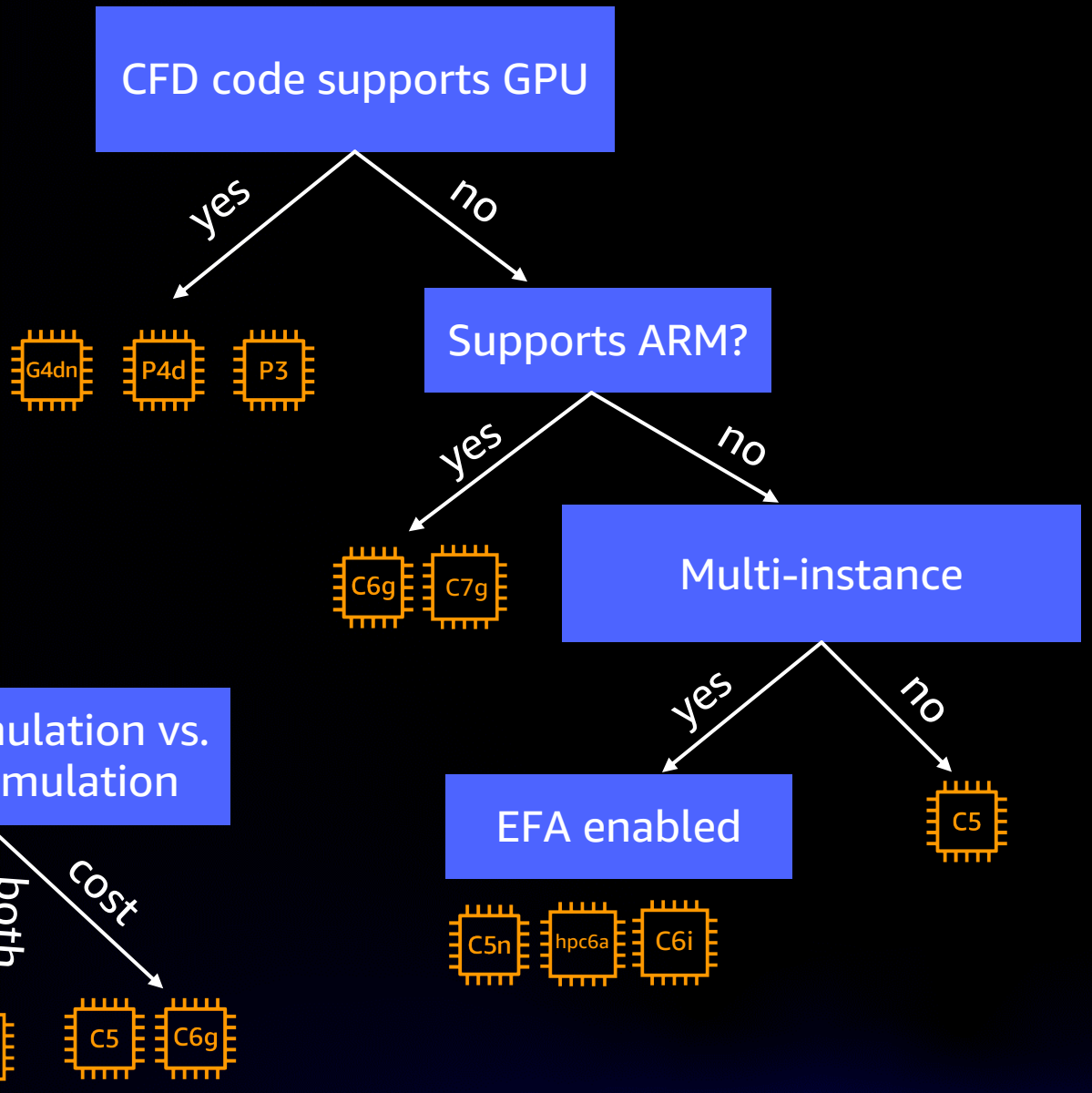
Instance type selection





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Amazon EC2 Hpc6a instances

Designed to deliver the best price performance for compute-intensive, high performance computing workloads in Amazon EC2

AMD 3rd Gen EPYC Milan processors, 96 cores, up to 3.6GHz frequency, and 384GB of RAM

Up to 65% better price performance over comparable Amazon EC2 x86-based compute-intensive instances

Elastic Fabric Adapter enabled by default for 100 Gbps networking for inter-instance communications

AWS Regions at launch: US East (Ohio) and GovCloud US West

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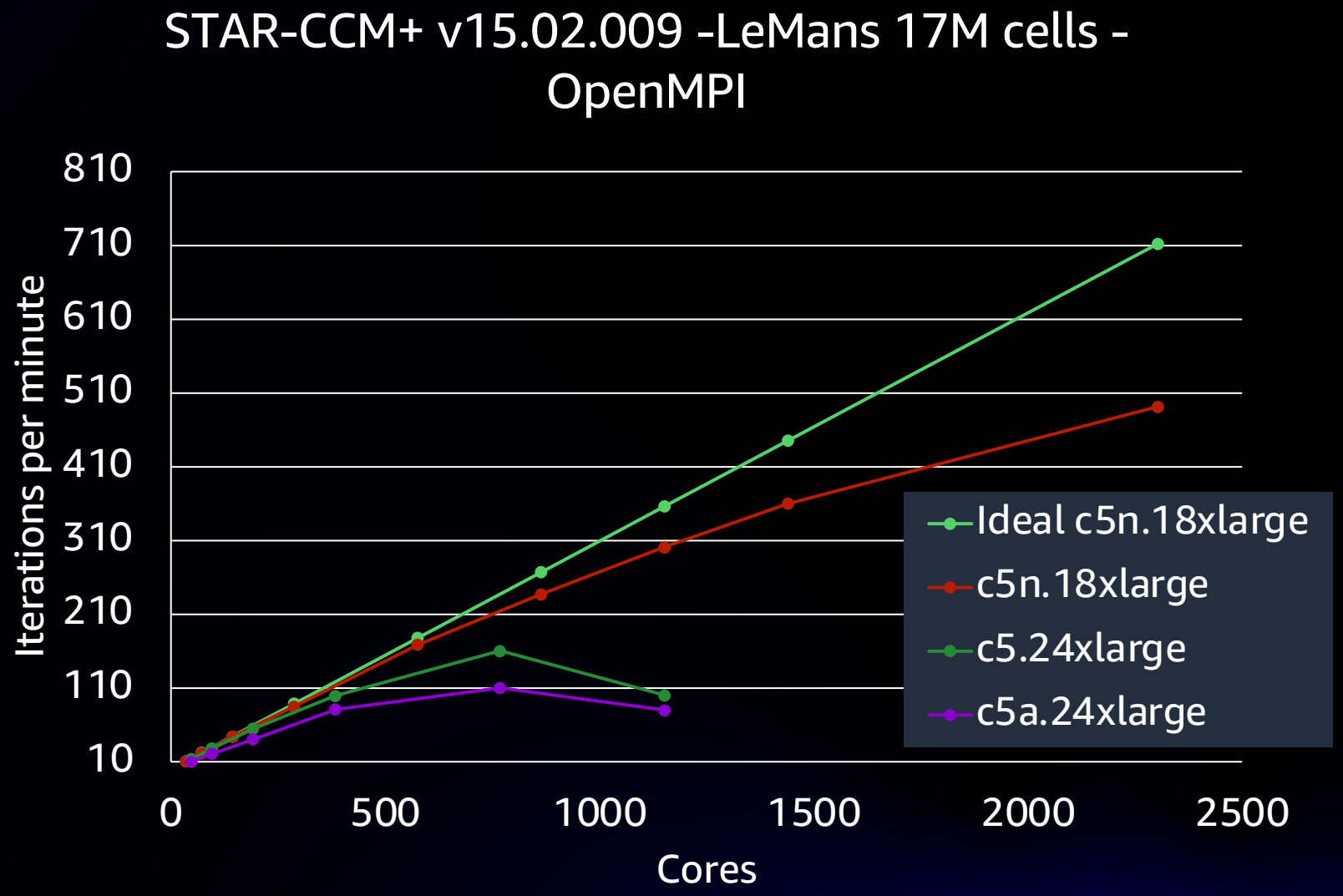
Multi-node

- For multi-node, the network bandwidth plays a key role
- CFD splits the solution into lots of partitions and then communicates the values around neighboring cells
- Key metric is cells per core



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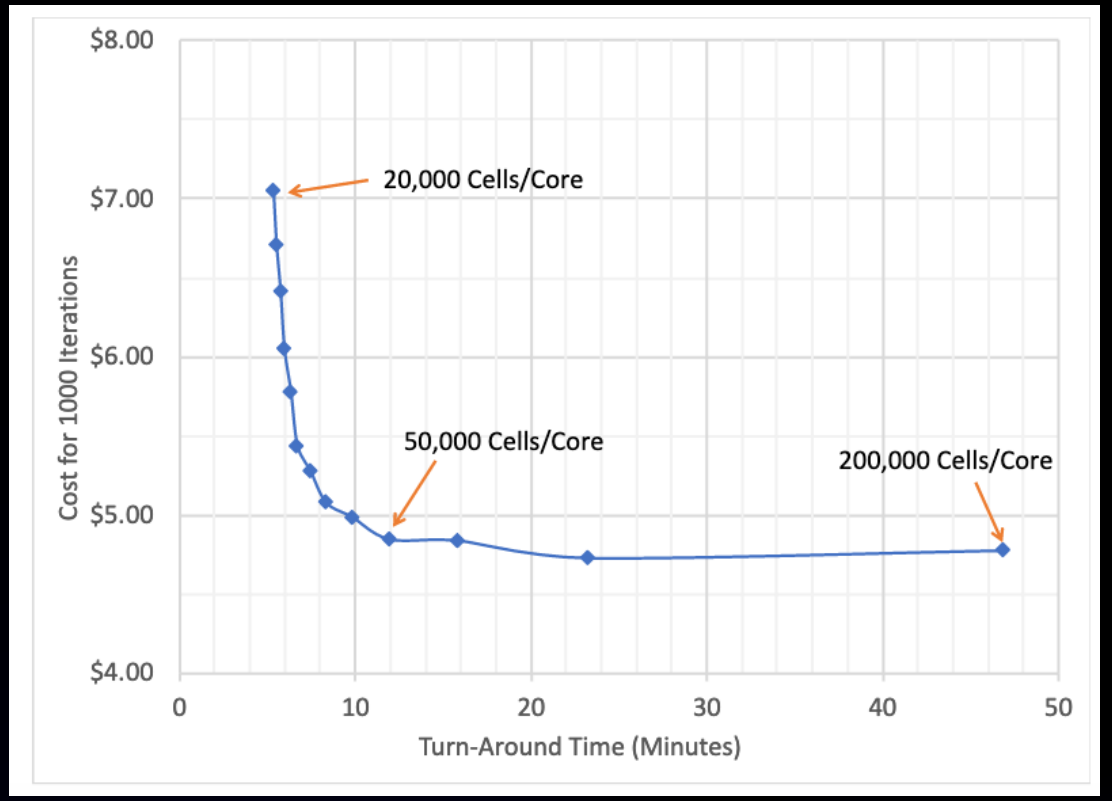
Cells per core

To achieve best parallel efficiency, we recommend greater than

50K cells/core



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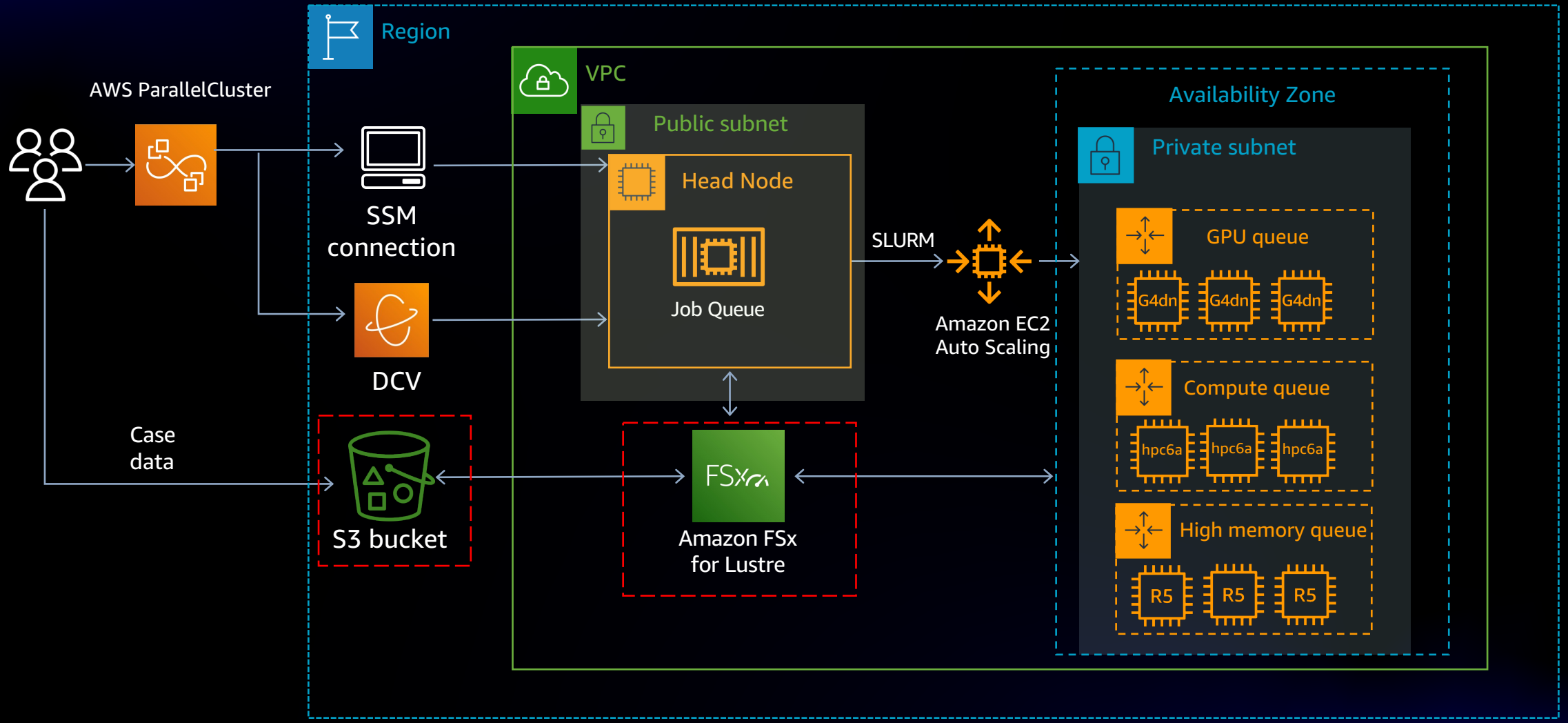
Reference architecture



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Storage options optimized for price performance

Storage type	Baseline throughput per TiB	Price per GB/s-hour
HDD Persistent	12 MB/s	$2.85
	40 MB/s	$2.85
NEW SSD Persistent	125 MB/s	$1.59
	250 MB/s	$1.15
	500 MB/s	$0.93
	1000 MB/s	$0.82

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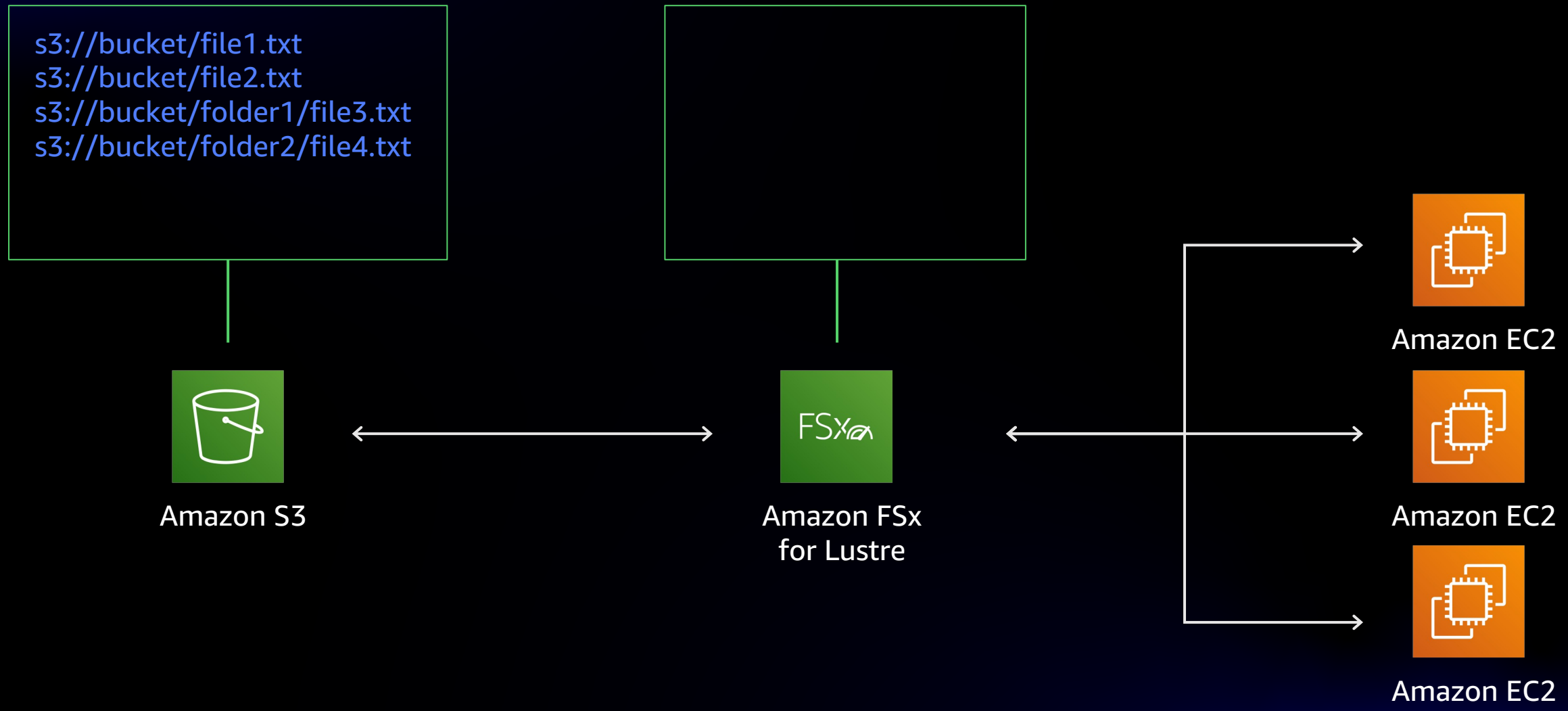
Fast file interface for data on S3: How it works



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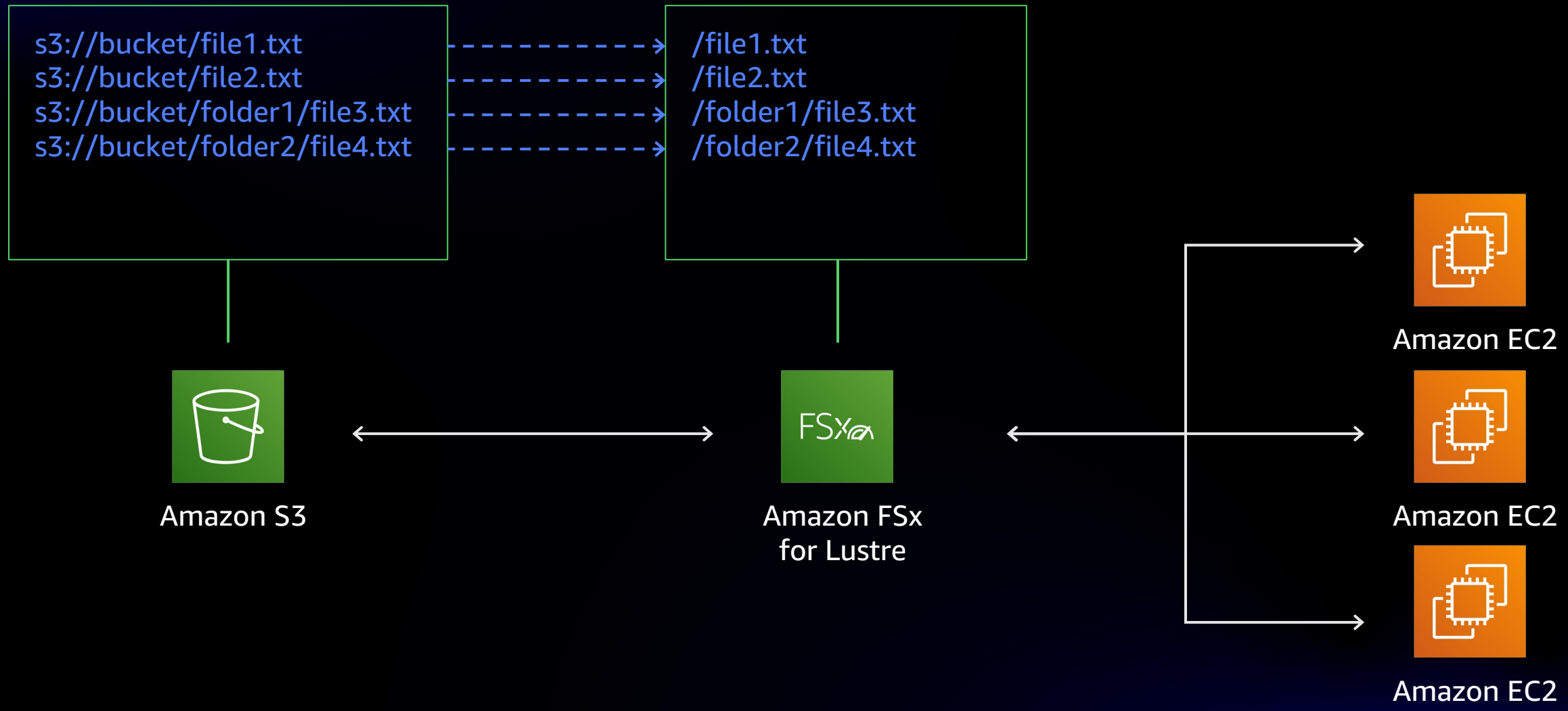
S3 objects appear on FSx file systems



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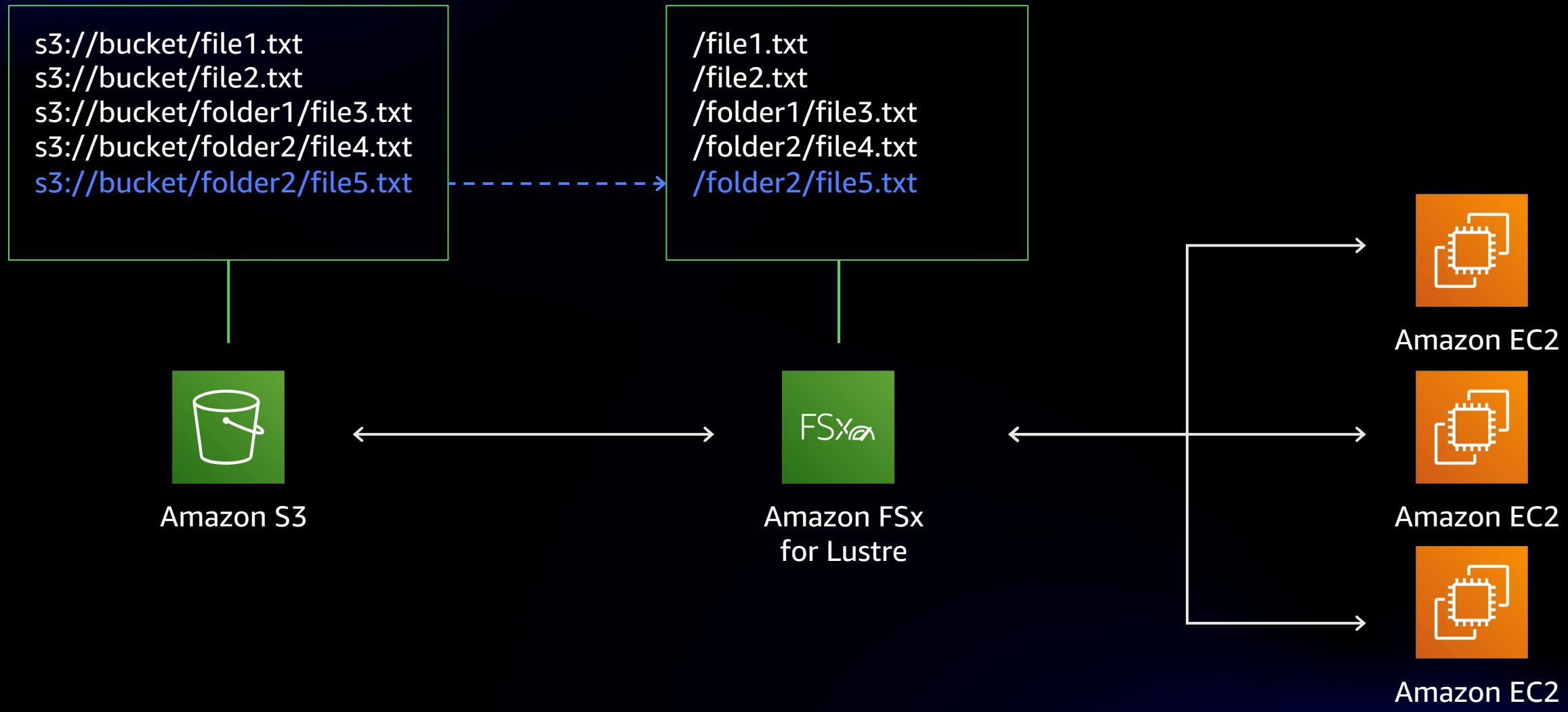
Updates on S3 are imported to FSx for Lustre



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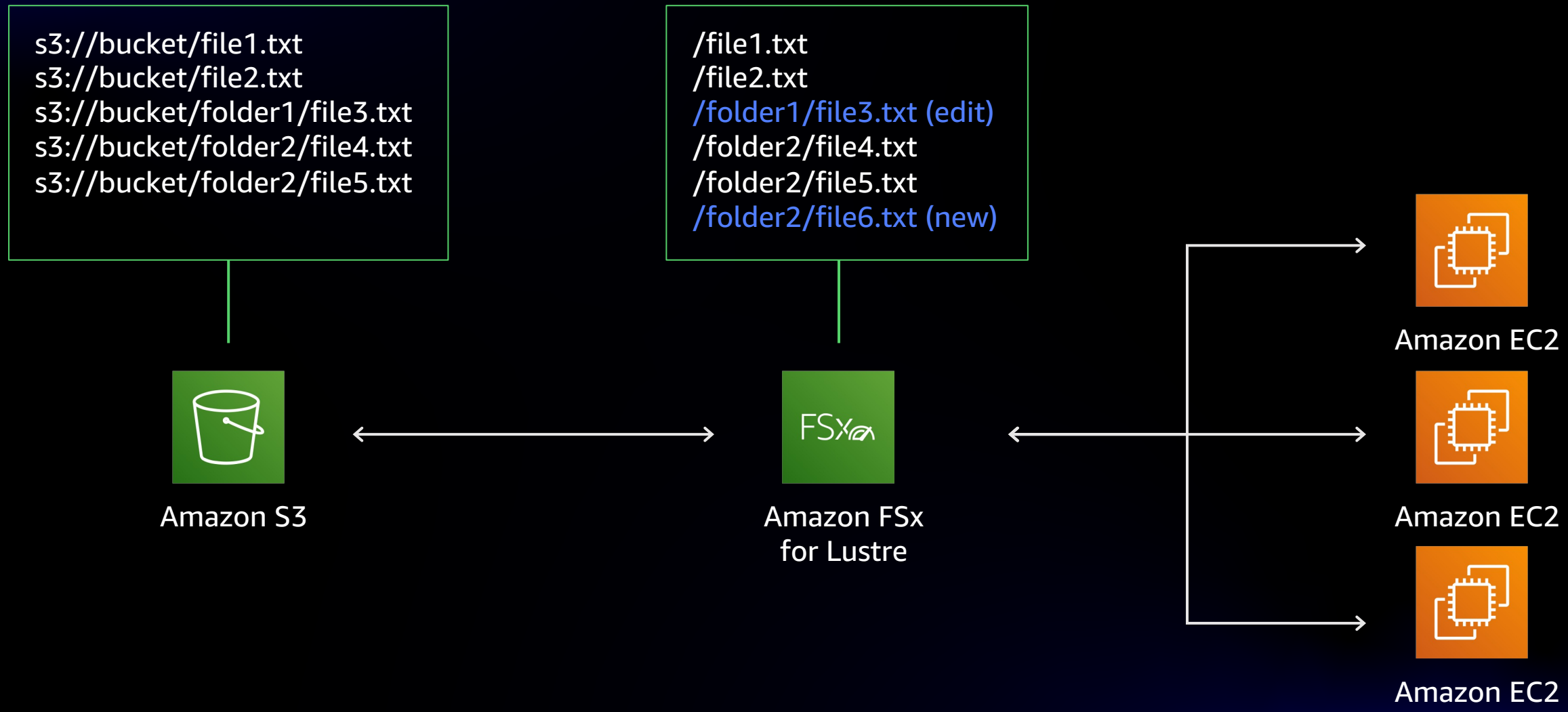
Updates on FSx for Lustre are exported to S3



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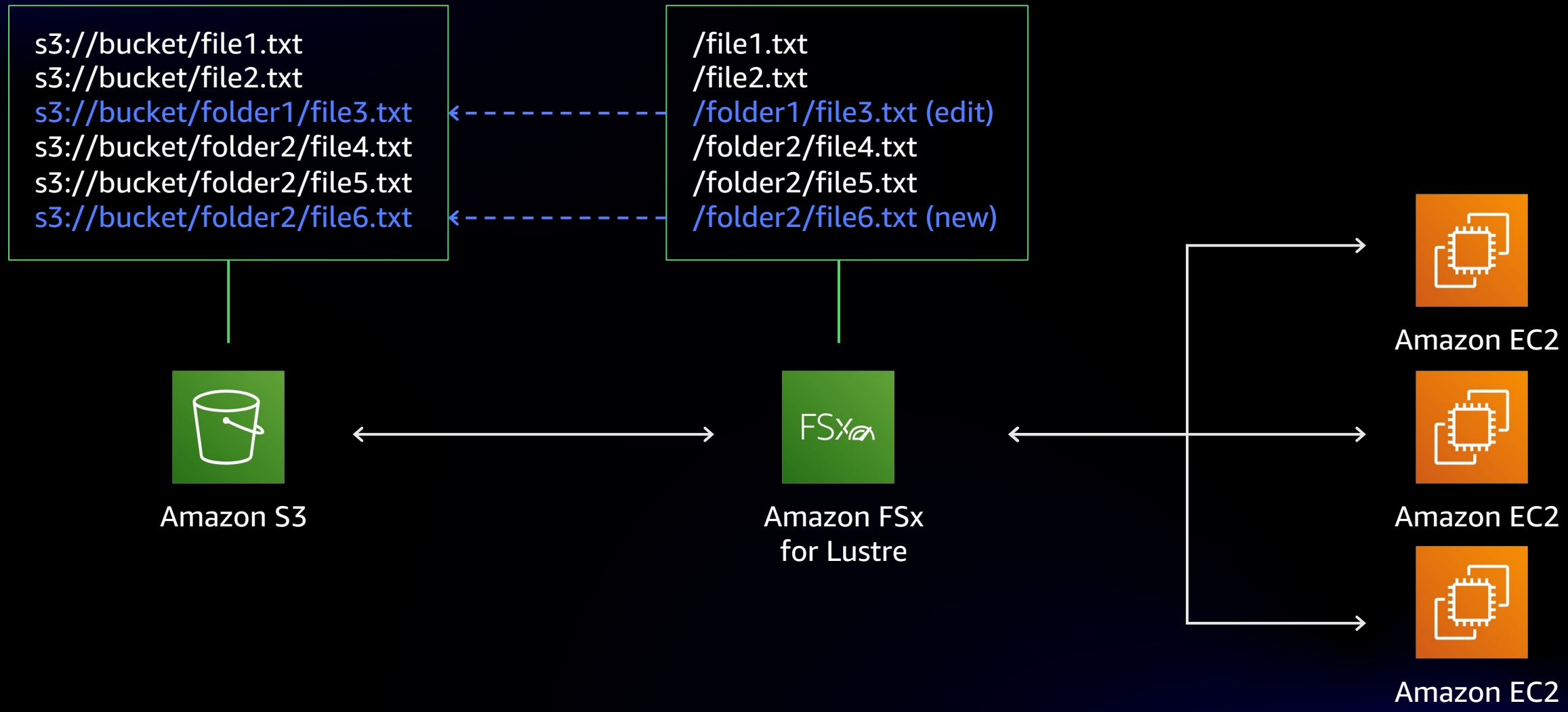
Updates on FSx for Lustre are exported to S3



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Spin up/spin down with compute resources

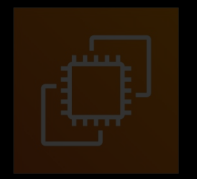
s3://bucket/file1.txt
s3://bucket/file2.txt
s3://bucket/folder1/file3.txt
s3://bucket/folder2/file4.txt
s3://bucket/folder2/file5.txt
s3://bucket/folder2/file6.txt

Amazon S3

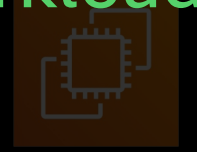
/file1.txt
/file2.txt
/folder1/file3.txt (edit)
/folder2/file4.txt
/folder2/file5.txt
/folder2/file6.txt (new)

Amazon FSx
for Lustre

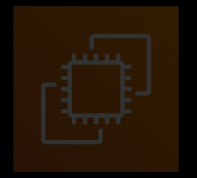
Spin down resources between workloads



Amazon EC2



Amazon EC2



Amazon EC2

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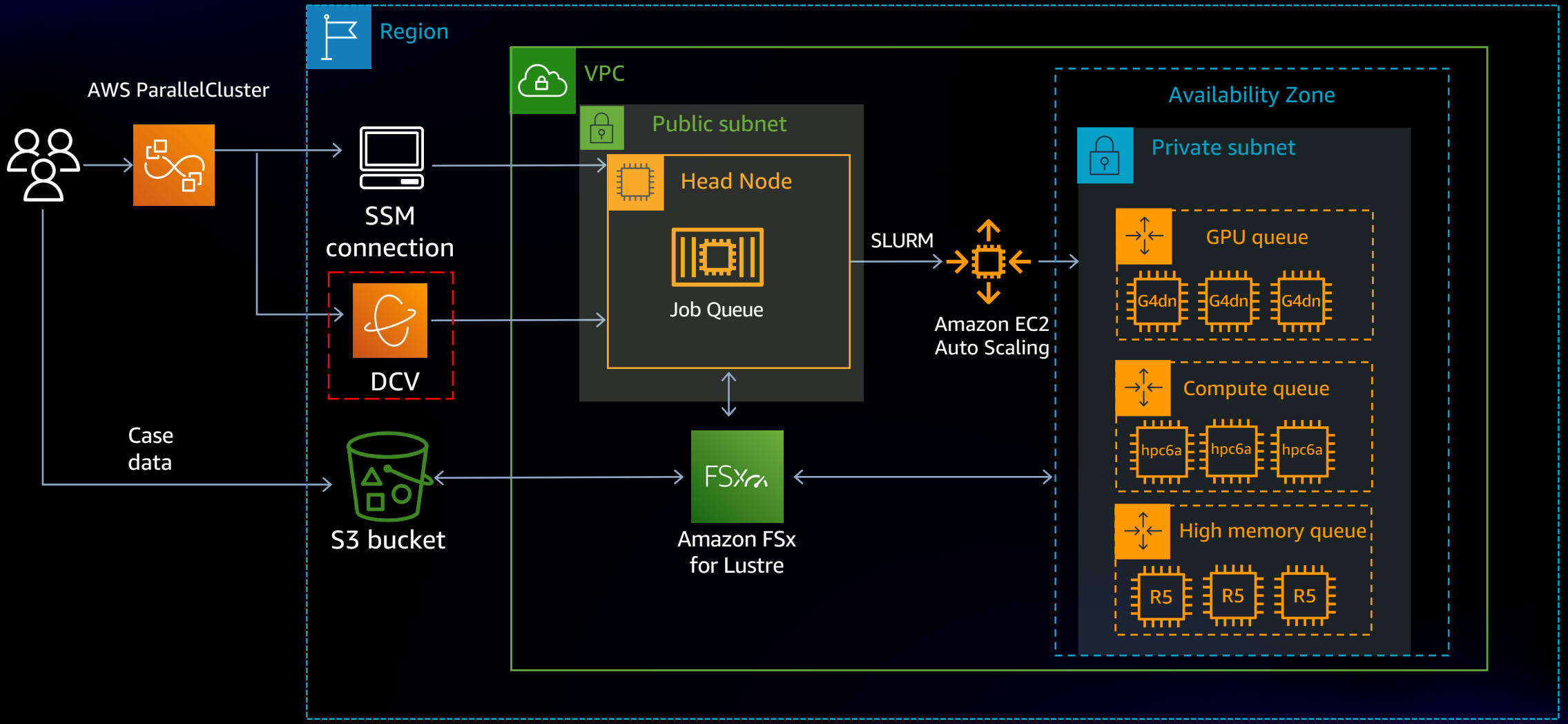
Reference architecture



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NICE DCV encrypts and transports pixels to devices

Users can access, manipulate, and share business-critical information, regardless of their location, over LAN or WAN networks

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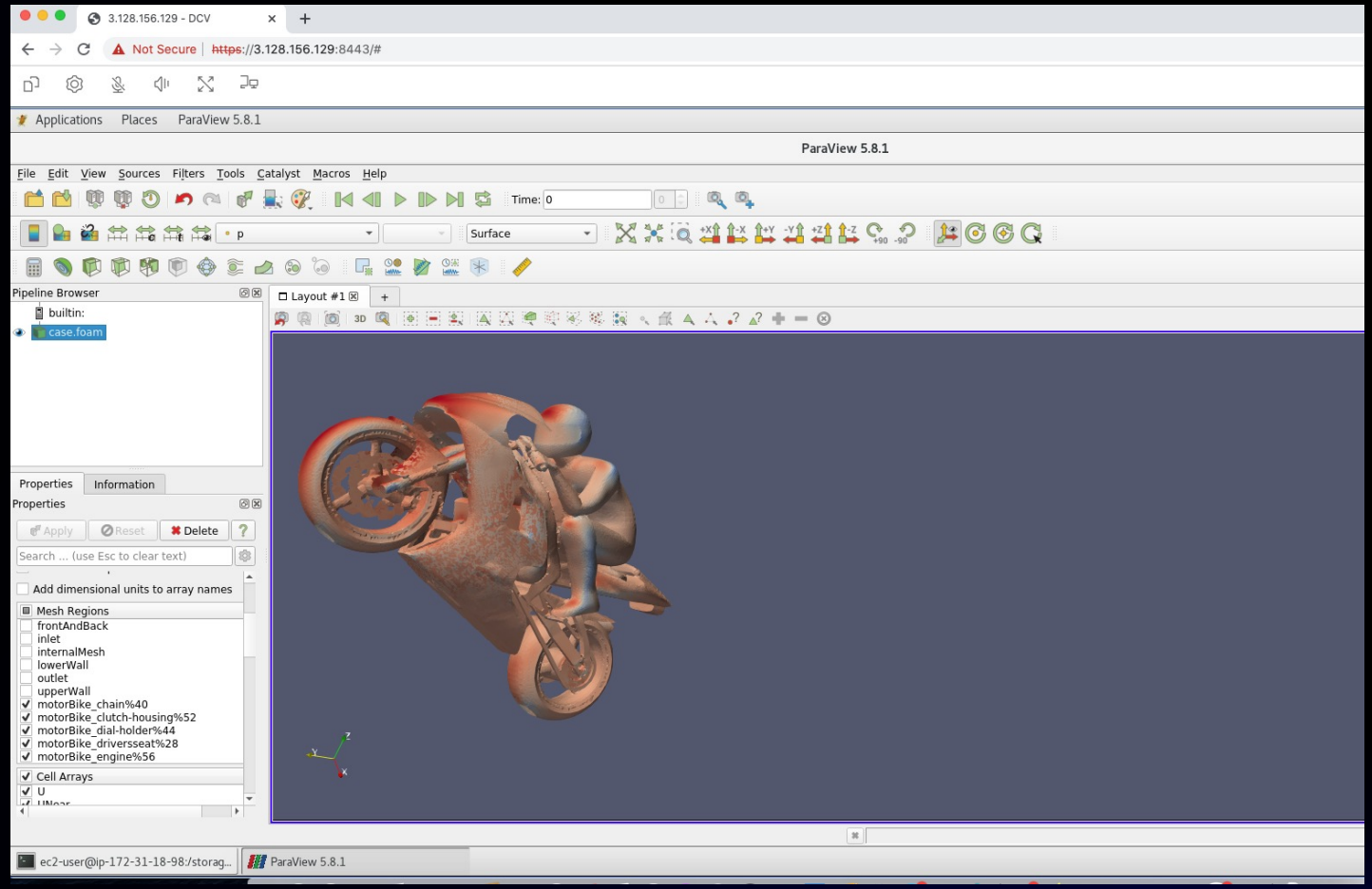
DCV enables pre & post processing in the cloud



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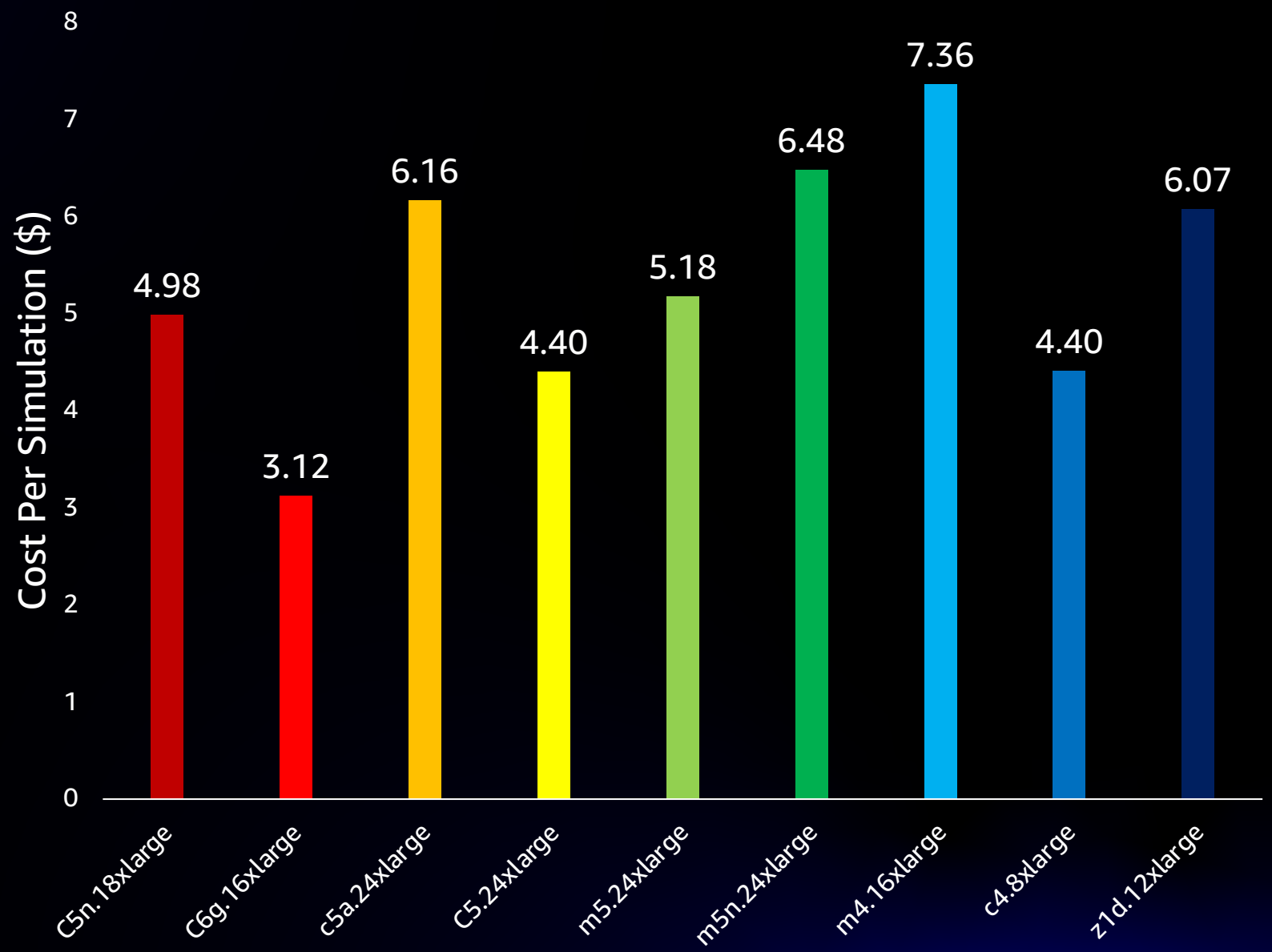
Instances

- Many users (especially commercial) want the best price/performance
- C6g.16xlarge is the clear winner who can use Arm – not all codes can support
- C5.24xlarge is still the best with c4.8xlarge an option but for x2 slower turnaround



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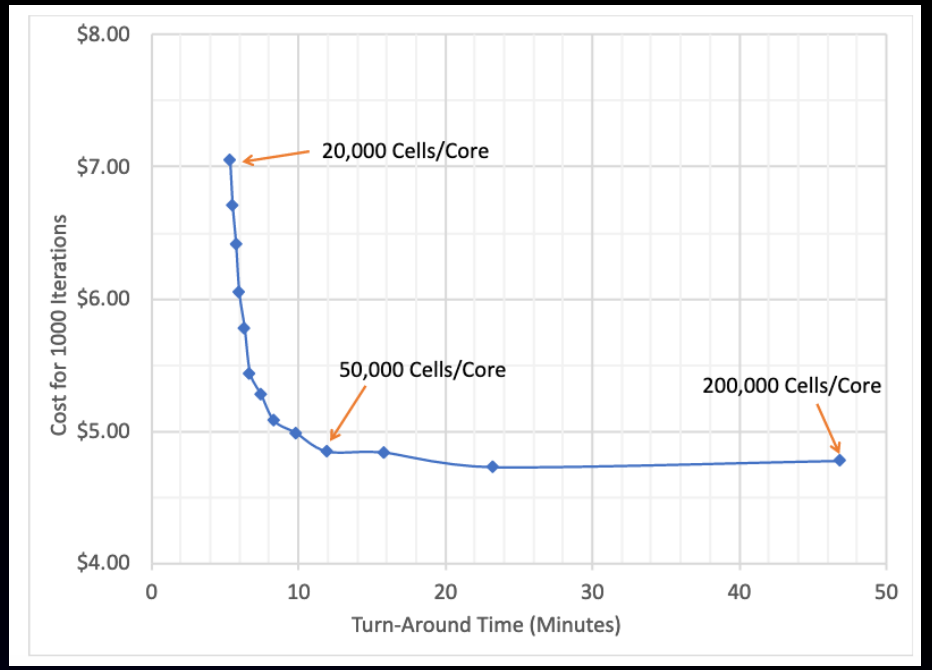
Time to solution vs. cost per simulation

- Optimize compute instance selection and number of instances
- Choose the optimal cells/core for your model
- Optimize storage by using FSx Lustre as scratch space and S3 for long term storage
- Next look at pricing models such as Spot or Reserved Instances

Evaluate the tradeoff of time to solution vs. cost for scaling



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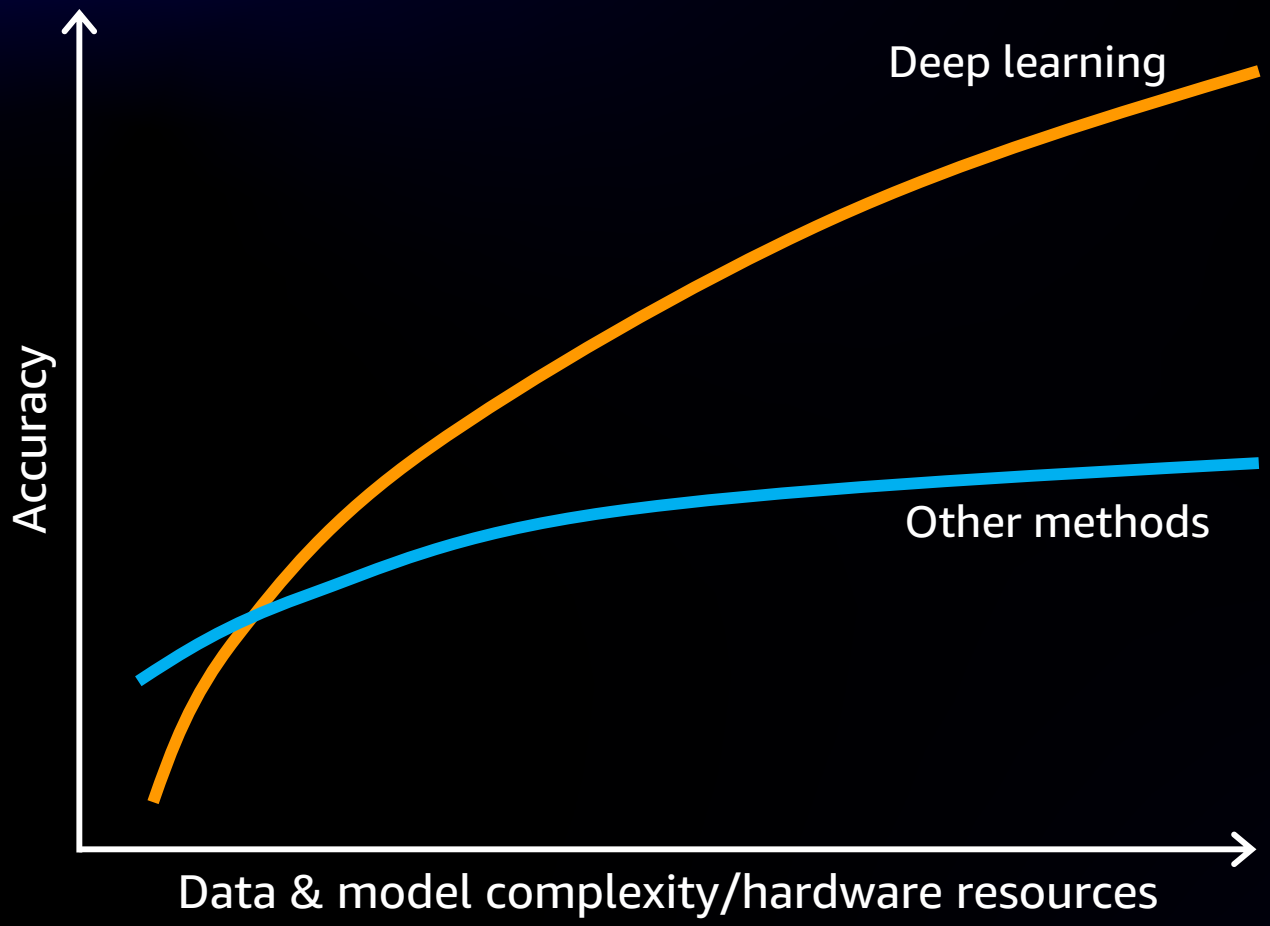
Innovating with ML



Applications

Natural language processing

Image/ video analysis

Autonomous vehicle systems

Recommendation systems

Model accuracy continues to increase with additional data

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Demonstrating ML + HPC:
Extract relationships from HPC simulation results

Problem statement

Determine optimal lead car features to obtain target flow profile at distance X

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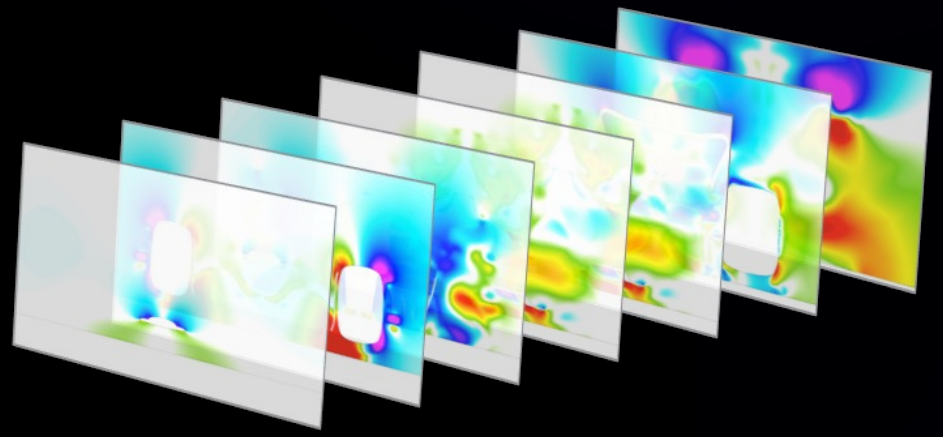
ML + HPC solution

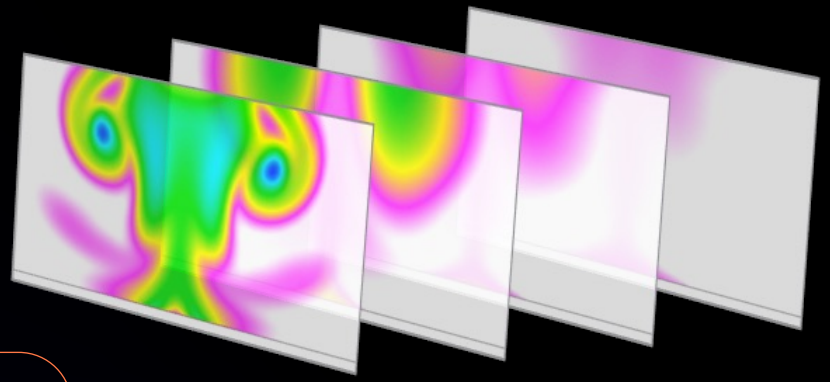
3D geometry

Input flow field

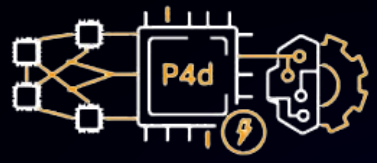
Deep learning model

Output flow field





EC2 UltraClusters



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Call to action

CMP324-R2: Scaling machine learning workloads on Amazon EC2
Date: Thursday, December 2, 1:00–2:00 PM
Location: Level 1, Alliance 311, Caesars Forum

CMP312: The future of HPC is looking a lot like ML
Date: Thursday, December 2, 3:15–4:15 PM
Location: Level 1, Summit 231, Content Hub, Blue Screen, Caesars Forum

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Key resources

CFD on AWS
aws.amazon.com/hpc/cfd

AWS CFD workshops
cfd-on-pcluster.workshop.aws

CFD on AWS whitepaper
d1.awsstatic.com/whitepapers/computational-fluid-dynamics-on-aws.pdf

Content is being actively developed – please check back frequently

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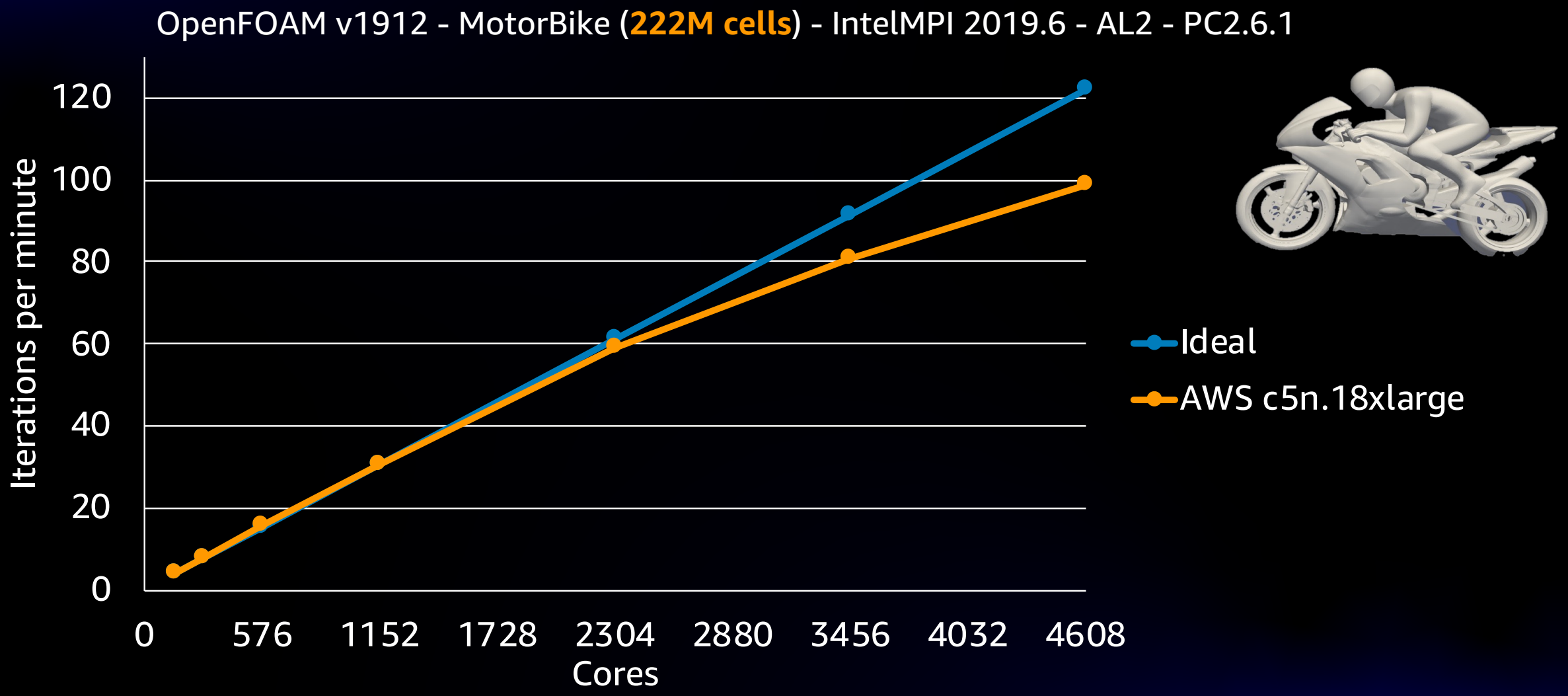
Scaling on AWS – OpenFOAM



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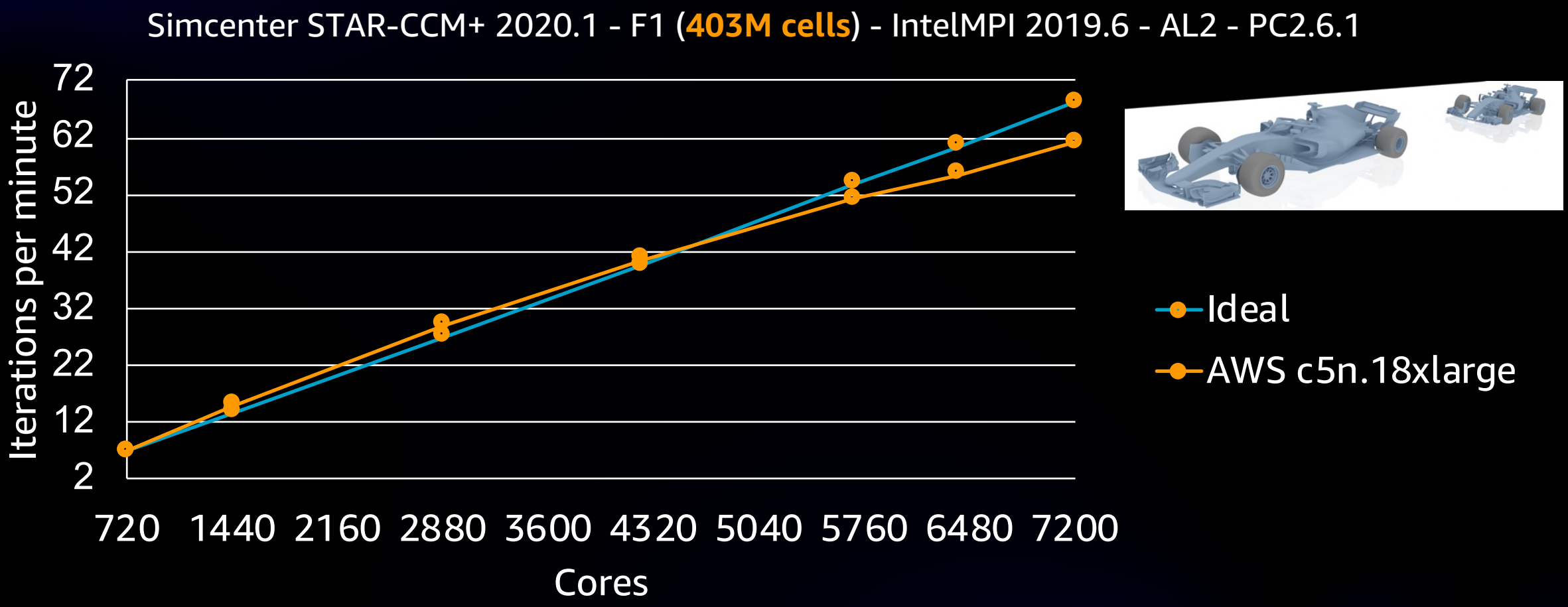
Scaling on AWS – STAR-CCM+



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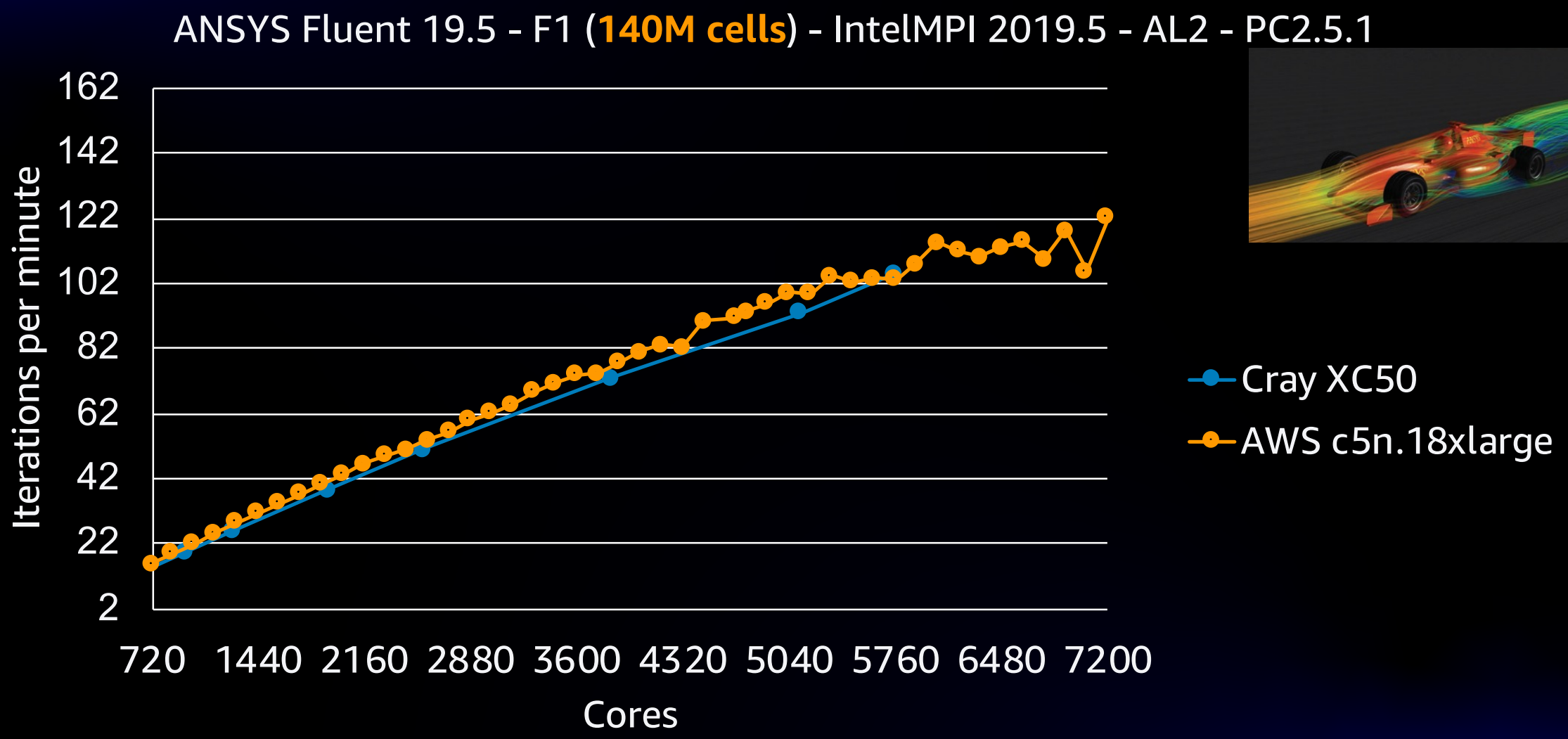
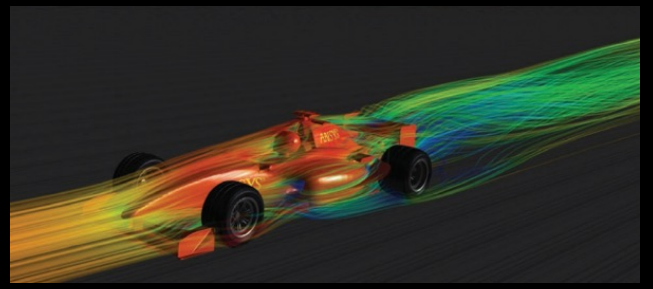
Scaling on AWS – Fluent





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