



# High Performance Computing Research on AWS

Solve complex problems with  
pay-as-you-go infrastructure

**Claudiu Farcas, PhD**  
AWS Principal Solutions Architect

20+  
years of  
**critical**  
research  
data

Is this  
you?



# Data is the new gold



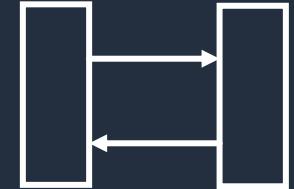
Documents  
Manuscripts



Databases /  
Repositories



Mobile and IoT  
Devices



REST/ APIs

Offline

Online



Tape  
Archives



Hard Drives,  
NAS Storage  
Appliances



Research  
Instrumentation



Web/ Cloud  
Storage

# Data-driven astronomy is here



New astronomical analysis increasingly relies on merging large and complex datasets in **computationally demanding** ways

**Geographically distributed** datasets

Researchers must be able to perform **customized queries** and analyses to answer **new questions**

Too much data!?



Space 1.0



Space 2.0



Space 3.0

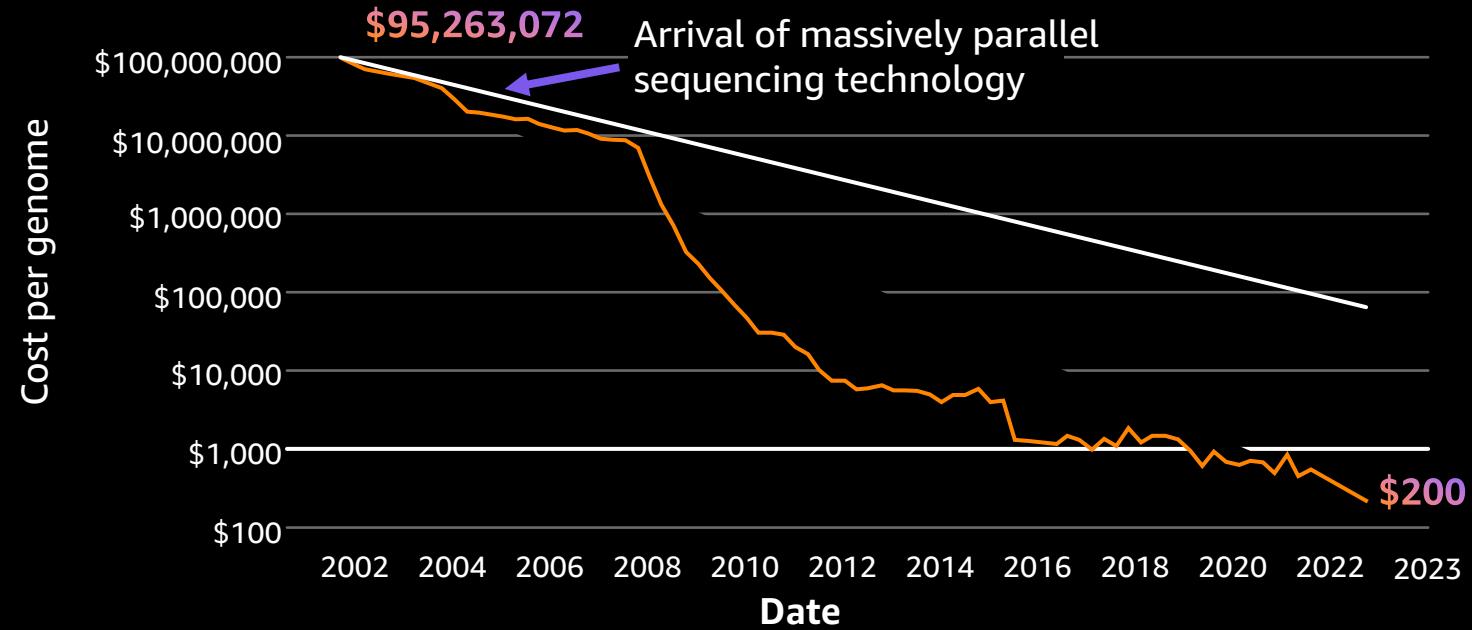


Space 4.0

# Genomics



A **deeper understanding** of biology has the potential to transform how we treat disease – but the **scale** and **complexity** of this data can create challenges



10s of millions of whole genomes sequenced and stored in the next five years

Requires multiple specialized tools and workflow languages

Need to combine numerous data modalities across silos

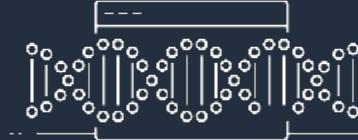
# HPC is all around us



Build designs faster  
with computational fluid  
dynamics (CFD) simulations



Fast-track drug  
discovery and structure-  
based drug design



Advance genomics insights  
using predictive, real-time, or  
retrospective data applications



Run geoscientific simulations  
and seismic processing  
and iterate models faster



Conduct grid-computing  
simulations and identify portfolio  
risks and hedging opportunities



Process complex workloads  
and analyze massive data  
pipelines to further research

# Community

- Regularly works on large problems, with diverse teams across dozens of institutions **around the world**
- Depends on, and contributes to, a **fast-evolving ecosystem of open-source software**, both within and beyond specific domains
- Wants to **focus on extracting the science**, not managing where the data are, whether the software is installed correctly, or how to manage permissions for collaborators



**Also, an old problem: The computation cannot always happen close to the data**

# Lost productivity and longer time to results

On-premises HPC infrastructure limits engineers, scientists, and researchers from getting timely results and insights to answer the world's biggest questions

**72.8%**

of organizations that use HPC reported delayed or canceled HPC jobs



## Lost innovation

Questions are left **unasked**, experiments are left **undone**, and potential revenue is **left** on the table



## Outdated technology

Almost **20%** of the useful life of new technology/hardware is **lost** in the procurement process



## Technical debt

Adapting **newer algorithms** to meet the requirements of an **existing infrastructure** = delays and **subpar performance**

Source: Hyperion Research



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# Why use the cloud?

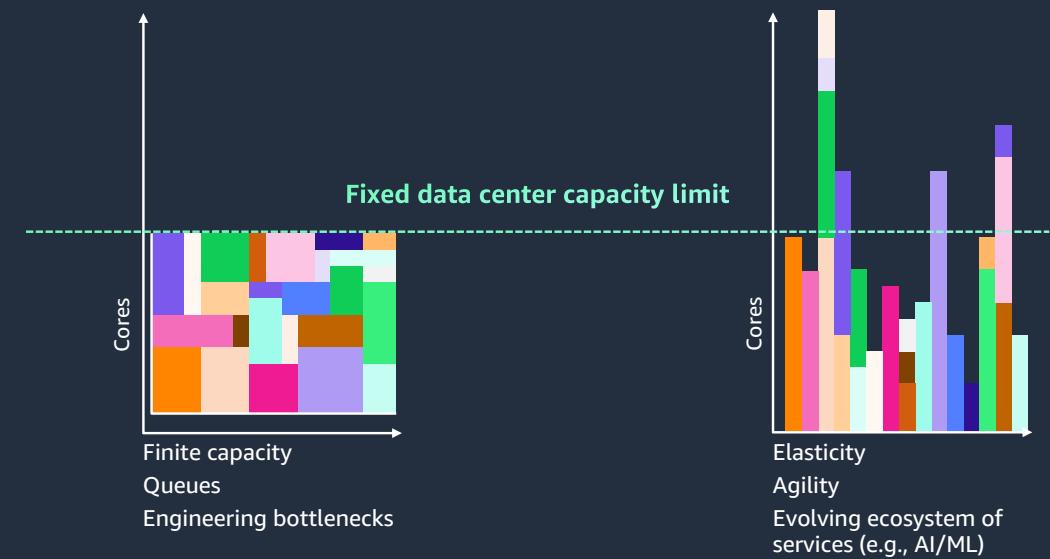
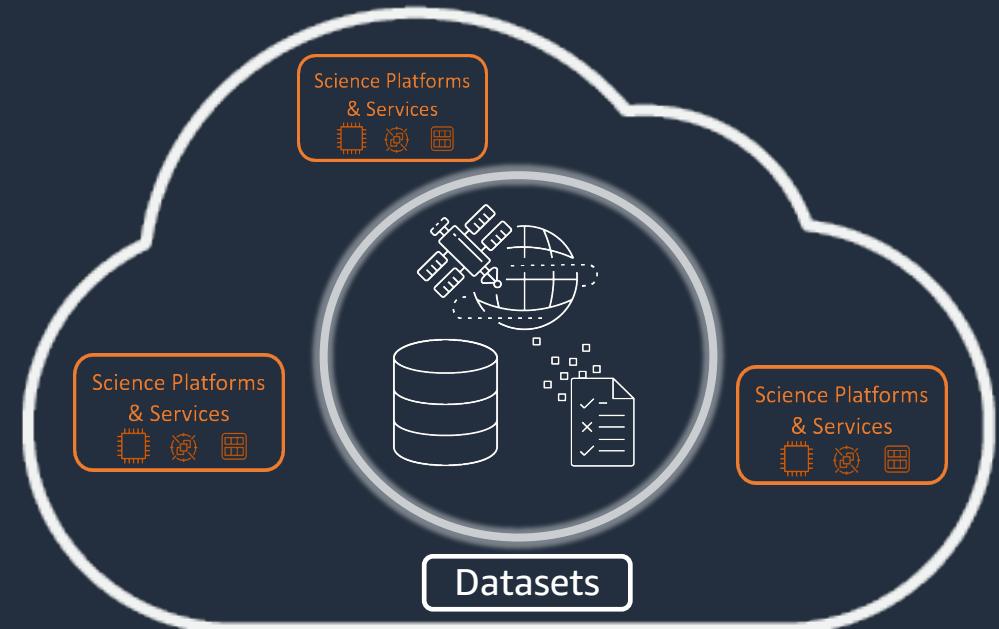
Large datasets can be **easily collocated** in the cloud

Cloud infrastructure naturally **locates compute next to the data**

Building science platforms and services around the data in AWS can easily use the **on-demand, scalable, and elastic compute** power of the cloud

Instant **access to latest technologies** with no lengthy procurement cycles or big capital investments

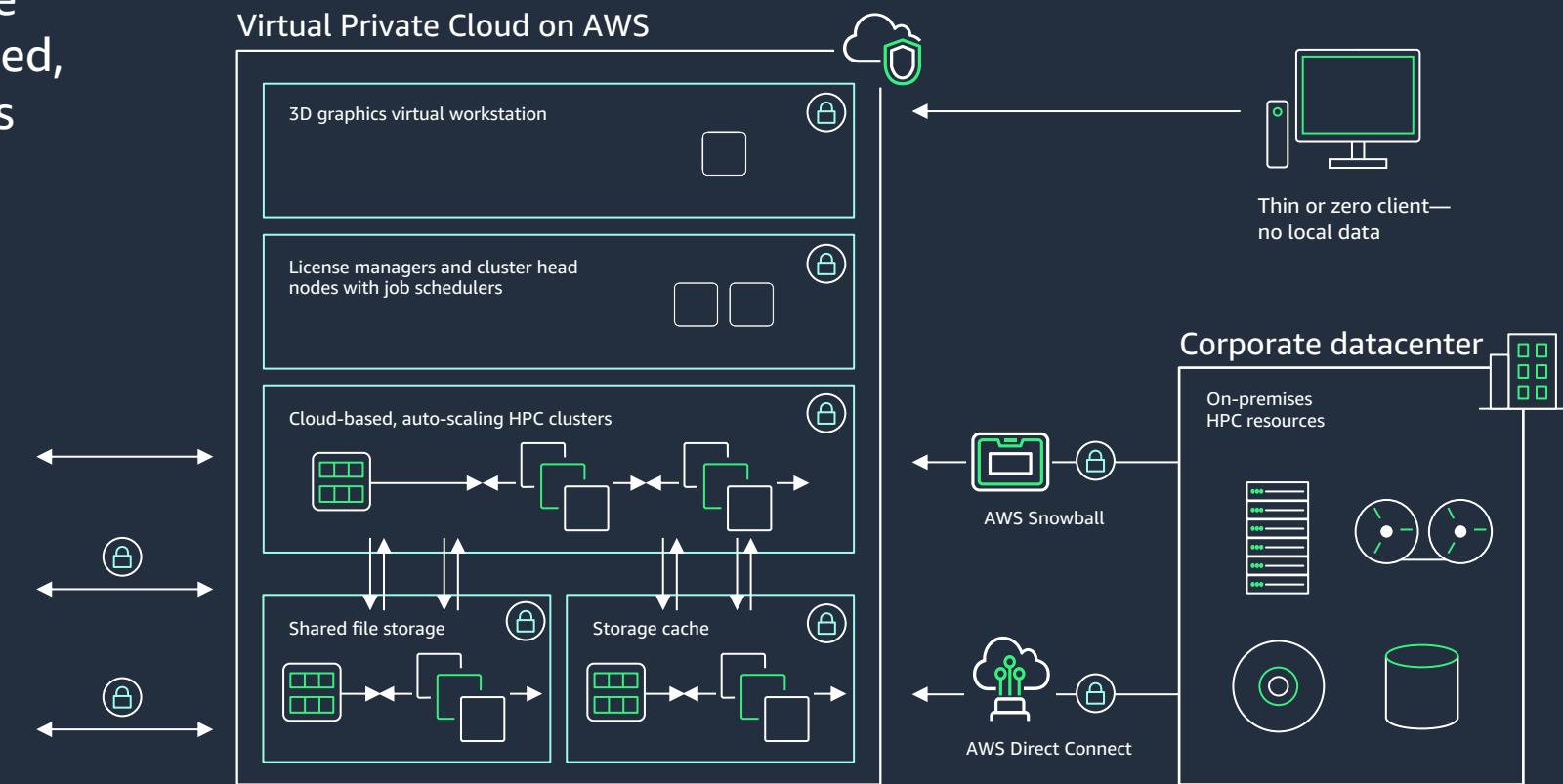
Well-built and maintained software environments are easy to support for the whole community in the cloud, enabling a **massive enhancement in scientific accessibility**



# High Performance Computing (HPC) on AWS

On AWS, secure and well-optimized HPC clusters can be automatically created, operated, and torn down in just minutes

- Machine learning and analytics
- Amazon S3 and Amazon Glacier
- Third-party IP providers and collaborators

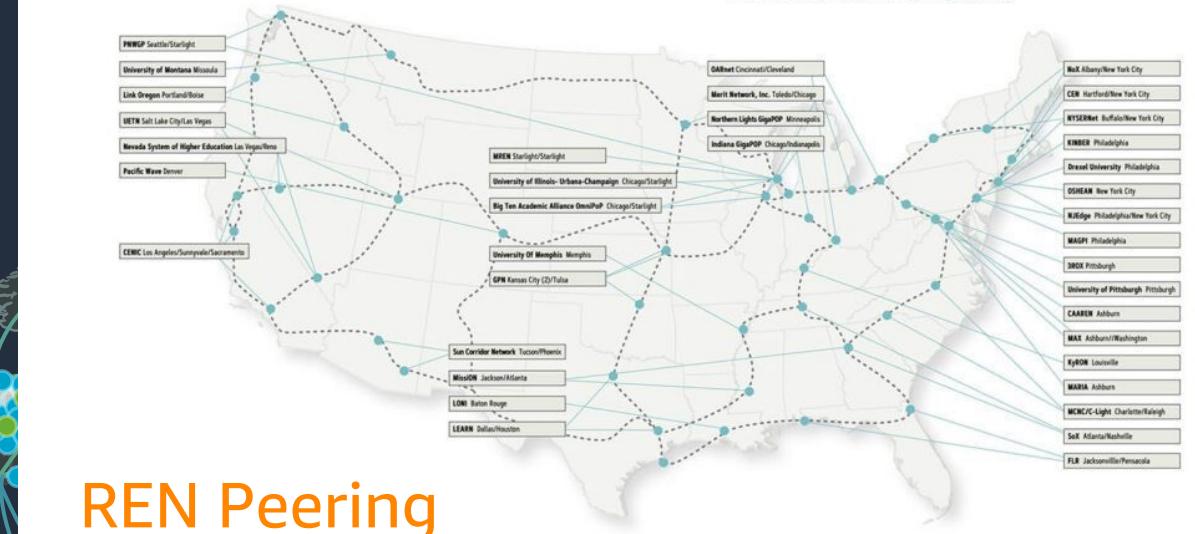


# AWS global footprint



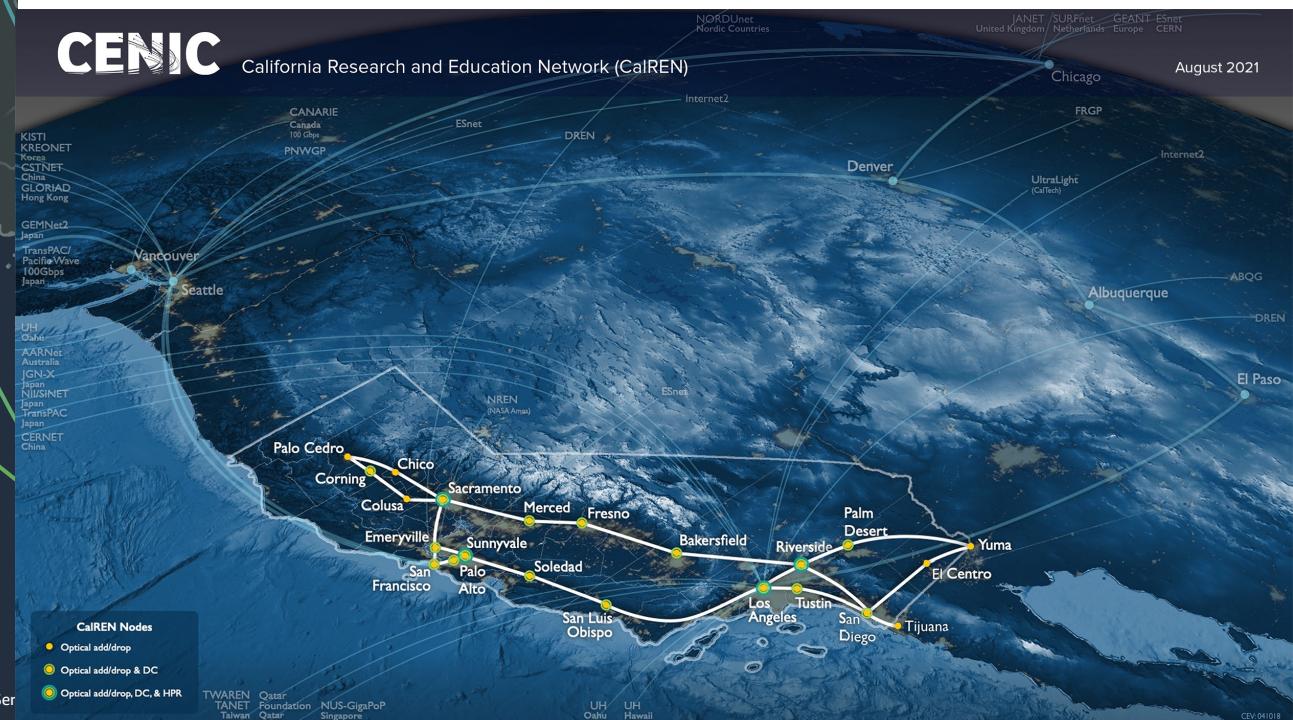
## Internet2 Network Connections

[internet2.edu/connectors](http://internet2.edu/connectors) 8.2022



CENIC

California Research and Education Network (CalREN)



# Global Data Egress Waiver

Why

Researchers need predictable budgets

- Available to degree-granting /research institutions
- Must use a research network (e.g. OARnet, Internet2) or AWS Direct Connect
- Worldwide (China Region excepted)

Who

Waives charges for data downloads over the internet

Capped at waiving up to 15% of the customer's bill

Data uploads are always free

What

Ask your AWS Account Manager

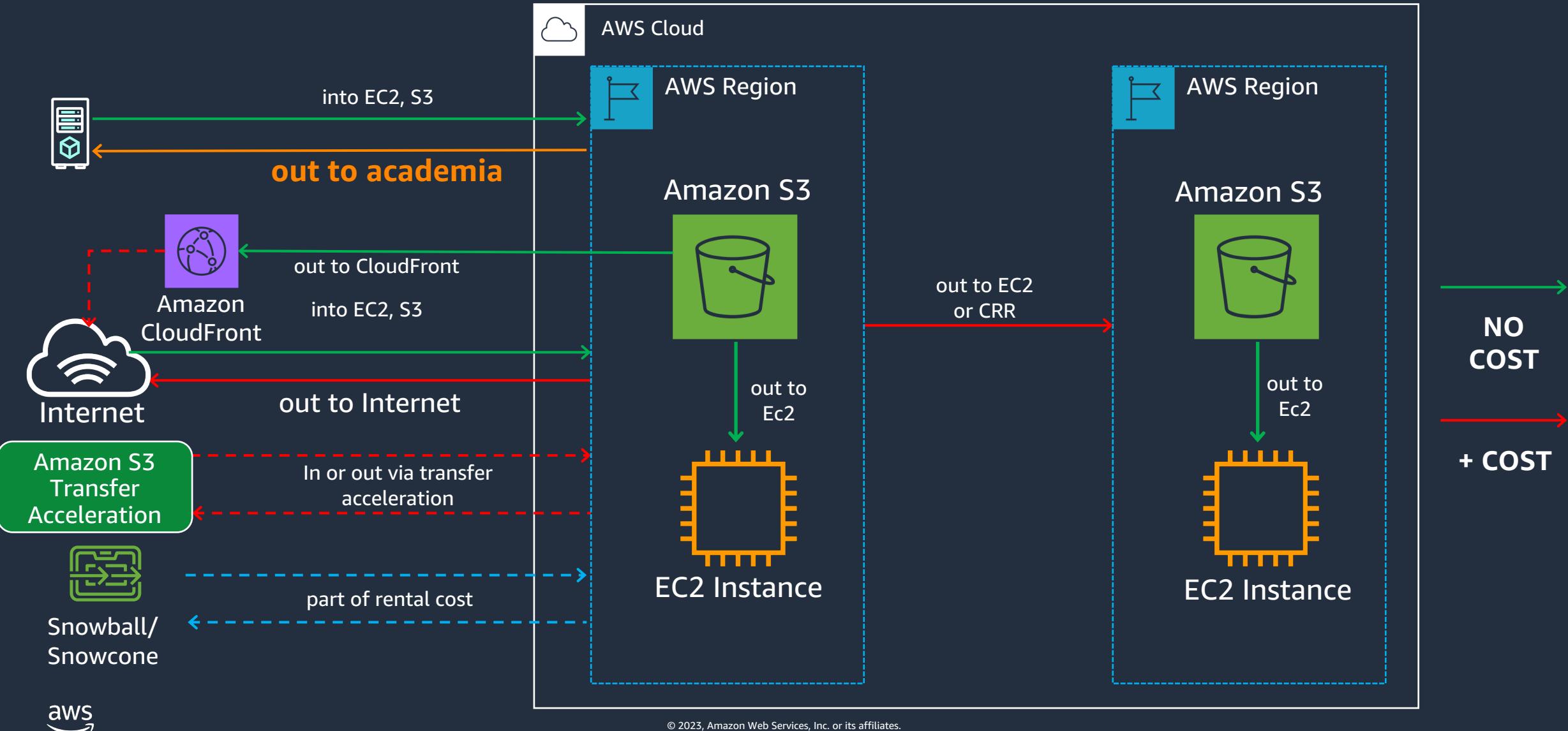
Or via Research Portals (e.g. Arcus, GEANT...)

Or via certain Resellers (e.g. DLT/I2 NET+, VMWare on AWS...)

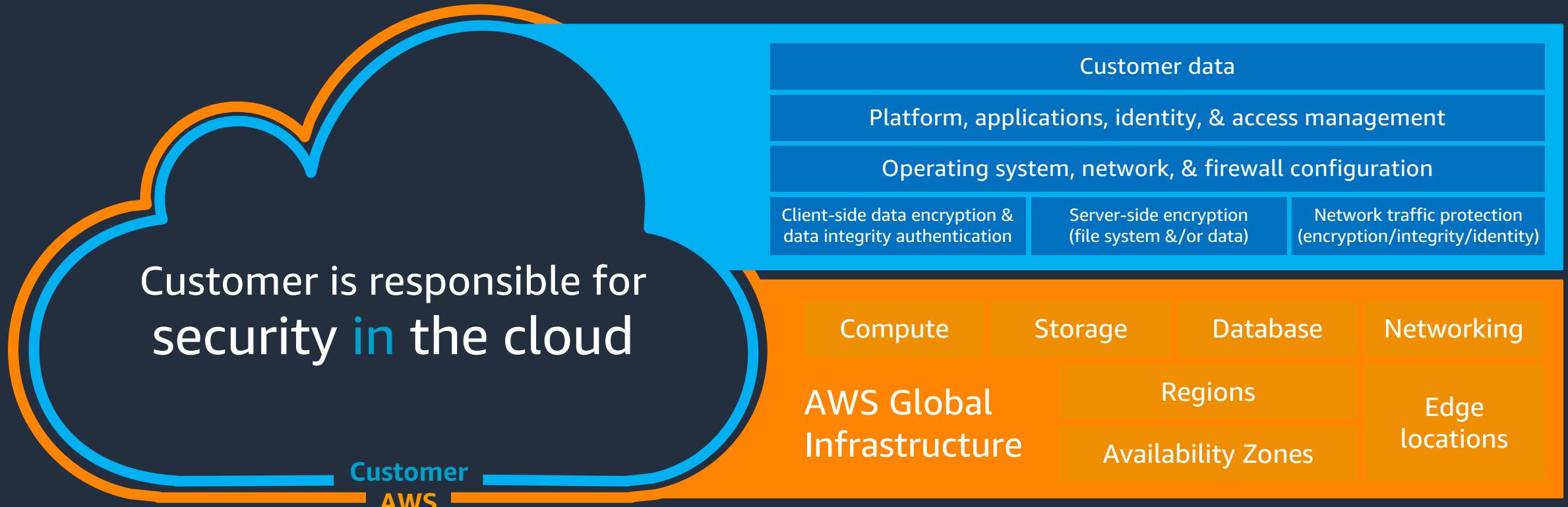
How



# Data Transfer Costs



# Shared security model



AWS is responsible for security **of** the cloud

# Compliance programs

Global  cloud security alliance



SOC 1



SOC 2



SOC 3



Europe



Asia Pacific



United States



# Shared operational responsibility model explained

More opinionated



## AWS manages

- Data source integrations
  - Application-level runtime and updates
  - Physical hardware, software, networking, and facilities
  - Provisioning
- 
- Container orchestration, provisioning
  - Cluster scaling
  - Physical hardware, host OS/kernel, networking, and facilities
- 
- Container orchestration control plane
  - Physical hardware software, networking, and facilities
- 
- Physical hardware software, networking, and facilities

## Customer manages

- Application code
  - Security and network configuration
- 
- Application code
  - Service scaling
  - Data source integrations
  - Security config, network config, management tasks, application runtime updates
- 
- Application code
  - Data source integrations
  - Worker hosts and service scaling
  - Security config and updates, network config, firewall, management tasks
- 
- Application code
  - Data source integrations
  - Instance scaling
  - Security config and updates, network config, management tasks
  - Provisioning, managing scaling and patching of servers

# Foundations of Research Computing/HPC on AWS

## Amazon CloudWatch

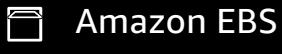
### Applications and Services

#### Automation and orchestration

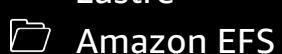


NICE EnginFrame

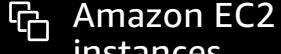
#### Storage



Amazon FSx for Lustre



#### Compute



Amazon EC2 Spot



#### Visualization



#### Networking

Enhanced networking

Placement groups

Elastic Fabric Adapter

## Amazon IAM (Identity and Access Management)

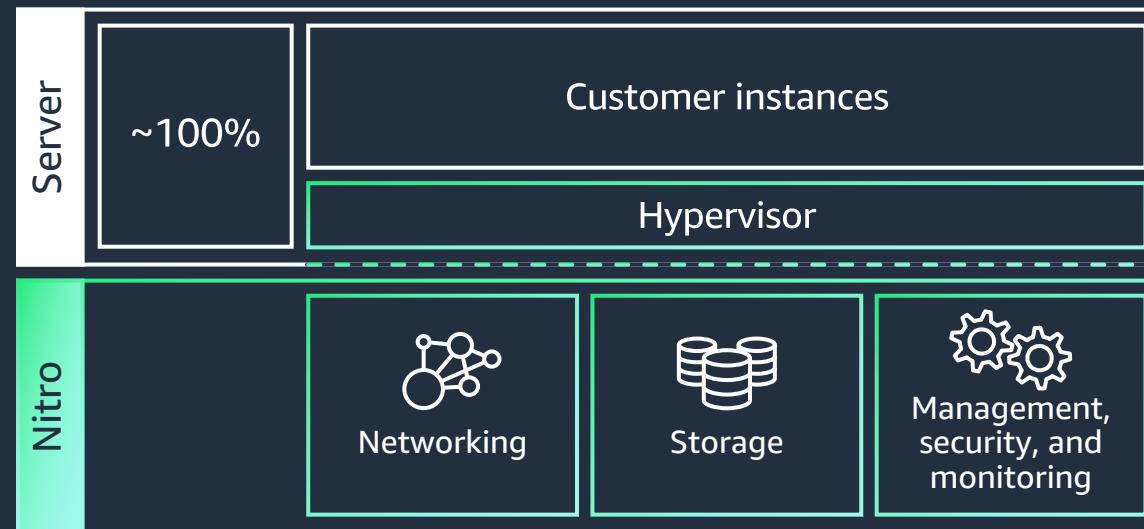
## AWS Budgets



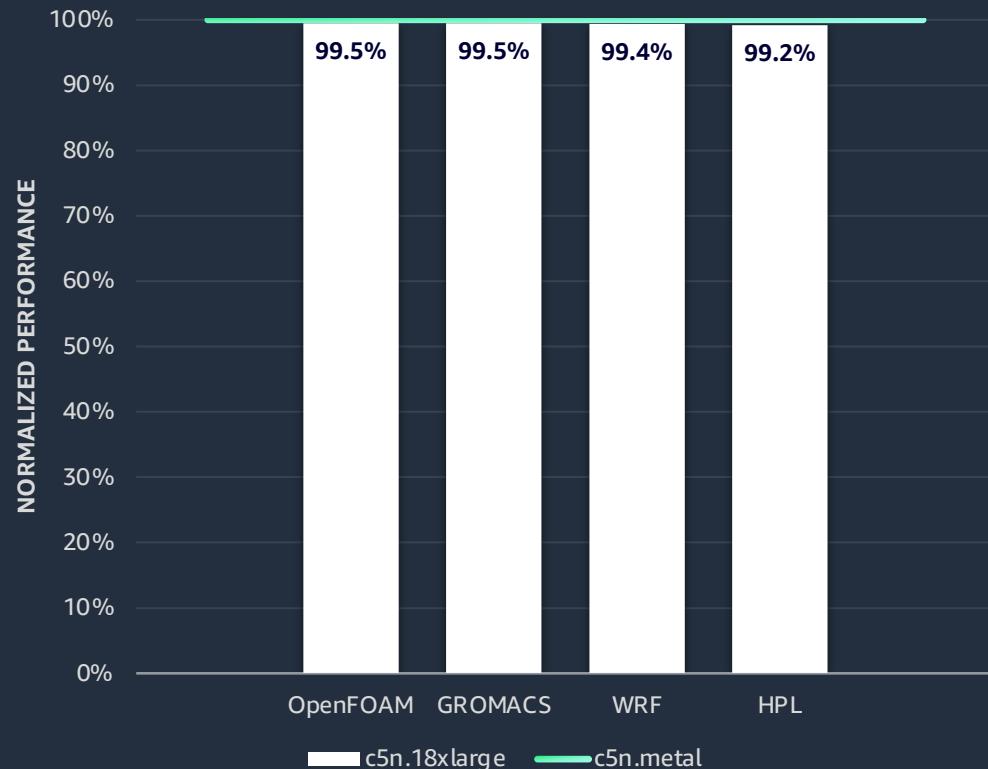
# The AWS Nitro System

The Nitro System lightweight hypervisor memory and CPU allocation are designed for **performance nearly indistinguishable from bare metal**

Designed using a security chip that monitors, protects, and verifies the instance hardware and firmware

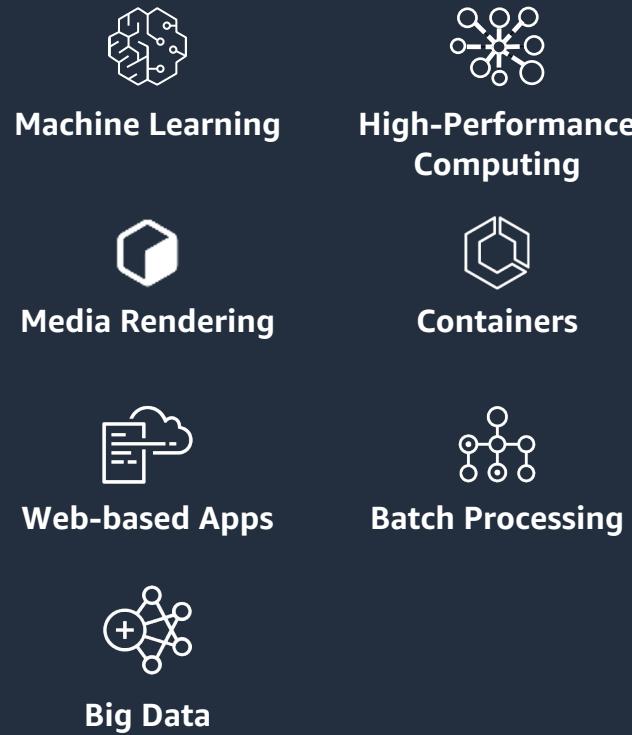


**Metal vs. Nitro Hypervisor**  
(16 instances)

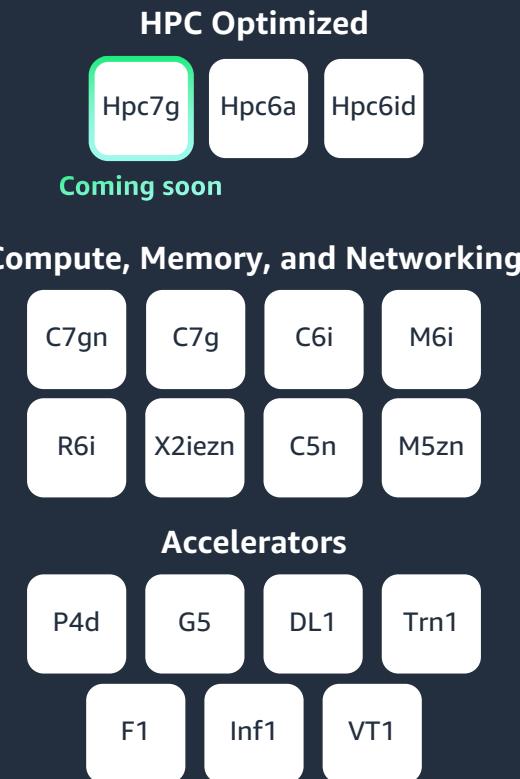


# Amazon EC2 | The compute platform for every workload

## Workload types



## Instance types for HPC workloads



## Scale tightly and loosely-coupled HPC applications

- Choice of processor (e.g., Graviton, Intel, AMD)
- Scale tightly-coupled HPC and ML workloads
- Up to 400 Gbps network bandwidth
- < 15 micro-seconds network latencies
- Accelerators use hardware to perform functions more efficiently than is possible in software running in CPUs

# Example: c5n high bandwidth compute

Massively scalable performance

- C5n Instances will offer up to 100 Gbps of network bandwidth
- Significant improvements in maximum bandwidth, packet per seconds, and packets processing
- Custom designed Nitro network cards
- Purpose-built to run network bound workloads including distributed cluster and database workloads, HPC, real-time communications and video streaming

Featuring

Intel Xeon Scalable  
(Skylake) processor



Instance Family

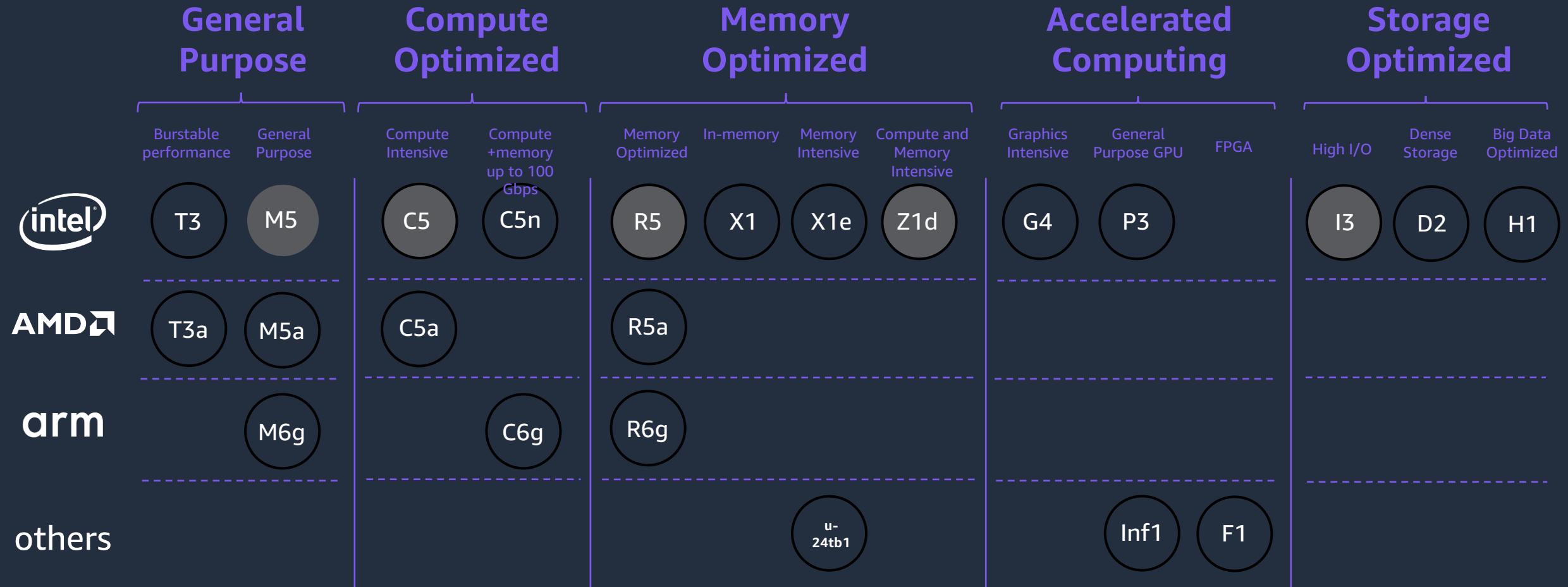
Type	Generation	Vendor/Features	Sizing
c5n.???			

Compute optimized  
1 vCPU : 2GB RAM

Intel Skylake/Cascade Lake

Elastic Fabric Adapter  
100Gbps

# EC2 Instance Types Explained



# AWS instance mapping to Nvidia GPUs

AWS instance/ NVIDIA GPU (professional grade):

Amazon EC2 P2	Amazon EC2 G3	N/A	Amazon EC2 P3	Amazon EC2 G4	Amazon EC2 p4d
NVIDIA K80	NVIDIA M60	NVIDIA P100/40	NVIDIA V100 (16 GB)	NVIDIA T4	NVIDIA A100 (40 GB)
			Amazon EC2 P3dn	Amazon EC2 G5g*	Amazon EC2 P4de
			NVIDIA V100 (32 GB)	NVIDIA T4g	NVIDIA A100 (80 GB)
				* Based on AWS Graviton2 CPU	Amazon EC2 G5
					NVIDIA A10g
Kepler	Maxwell	Pascal	Volta	Turing	Ampere

NVIDIA GPU Architecture:



# HPC-optimized Amazon EC2 instances



Coming soon!



Powered by third-generation AMD EPYC processors

## Amazon EC2 Hpc6a instances

Compute-intensive applications like Computational Fluid Dynamics and Numerical Weather Prediction

3.6Ghz 96 cores AMD Milan  
384GB RAM  
100Gbps EFA

Powered by third-generation Intel Xeon Scalable processors

## Amazon EC2 Hpc6id instances

Memory-bound and data-intensive workloads like Finite Element Analysis and seismic simulations

3.5Ghz 64 cores Intel IceLake  
1024GB RAM | 15.2TB NVMe  
200Gbps EFA

Powered by the next generation AWS Nitro System

## Amazon EC2 Hpc7g instances

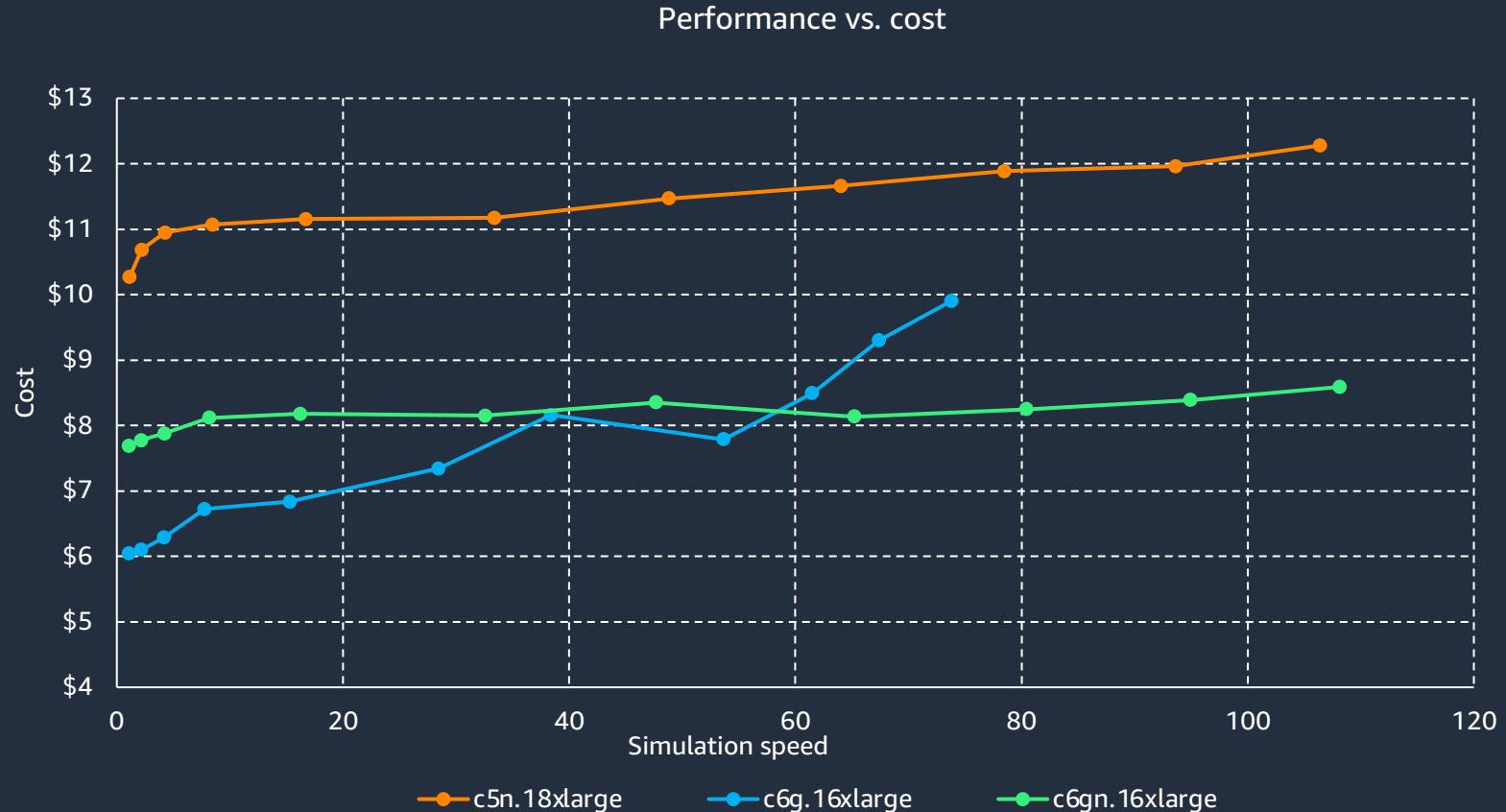
Based on custom AWS Graviton3E processors with low latency, and high network performance for MPI-based applications

2.6Ghz 64 cores Graviton3E  
128GB RAM  
200Gbps EFA



# C6gn price-performance for weather research forecasting simulations

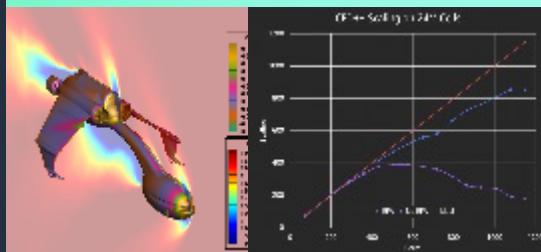
Scaling out the simulation to 112 nodes for each instance type C6g and C6gn are 40% and 30% less, respectively, compared to C5n. C6gn is the most performant at the least cost.



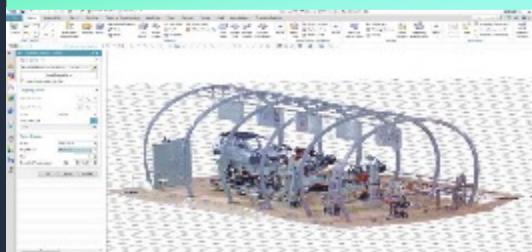
# Flexible compute options and purchase models optimize price performance

## Flexible compute to maximize performance

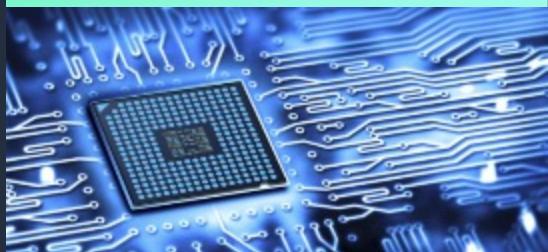
### Memory & compute optimized



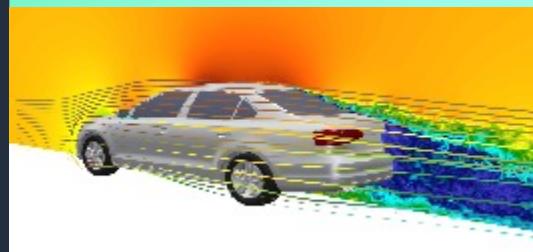
### Graphics and rendering



### High clock speed



### Accelerated computing



## Flexible pricing models to optimize cost

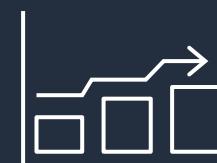
### On-demand

Pay for compute capacity by the second with no long-term commitments



### Savings Plan & Reserved Instances

Make a commitment and to save up to 72% off compute



### Spot Instances

Spare EC2 capacity at savings of up to 90% off On-Demand prices



# Ideal Spot workloads



Fault tolerant



Flexible



Loosely coupled



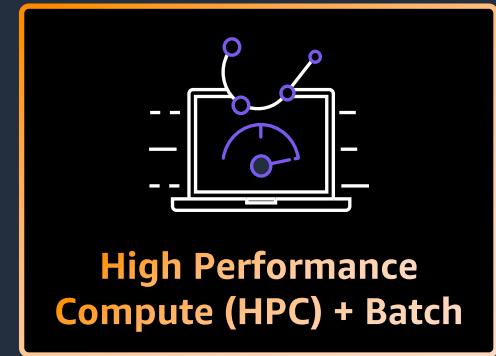
Stateless



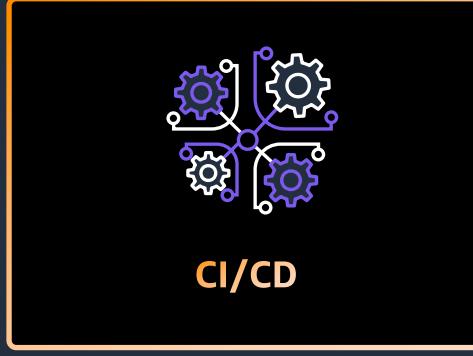
Web services



Containers



High Performance Compute (HPC) + Batch



CI/CD



Big data



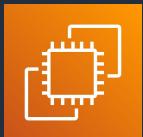
AI/ML

# Spot integrates easily with your workloads

## Launch methods



EC2 Auto Scaling



EC2 Fleet



AWS CloudFormation

## Application tools



AWS Batch



AWS Thinkbox Deadline



AWS Elastic Beanstalk

## Service integrations



Amazon Elastic Container Service



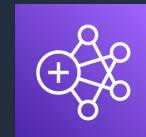
Amazon Elastic Kubernetes Service



AWS Fargate



Amazon SageMaker



Amazon EMR



**AWS Spot Blueprints** – dynamically provides reference architectures in CloudFormation and Terraform

## Spot ready partners



# What happens when AWS reclaims an instance?

## Minimal interruptions

Less than 5% of Spot instances were interrupted in the last 3 months



## EC2 Spot rebalance recommendation

An EC2 Spot Instance *rebalance recommendation* is a signal from that notifies you when a Spot Instance is at elevated risk of interruption. The signal can arrive *sooner* than the two-minute Spot Instance interruption notice, giving you the opportunity to proactively manage the Spot Instance.



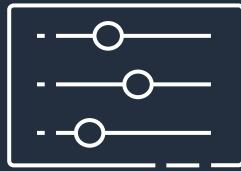
## Handling Options

- Terminate
- Stop/Start
- Hibernate

## Map to Strategy

# Flexibility is key to successful adoption

Instance  
flexible



- More than one instance type can get the job done
- Instance weighting gives you more flexibility on instance types
- Multiple instance types are key to resilient clusters

OR

Time  
flexible



Region  
flexible



Be time flexible to account for interruptions and/or location flexible to maximize application uptime

# Spot toolset

## Spot Blueprints

Dynamic infrastructure code generator



## Attribute-based instance selection

Provision capacity on instance attributes (such as CPU/Memory)  
Supporting new instances as soon as they become available

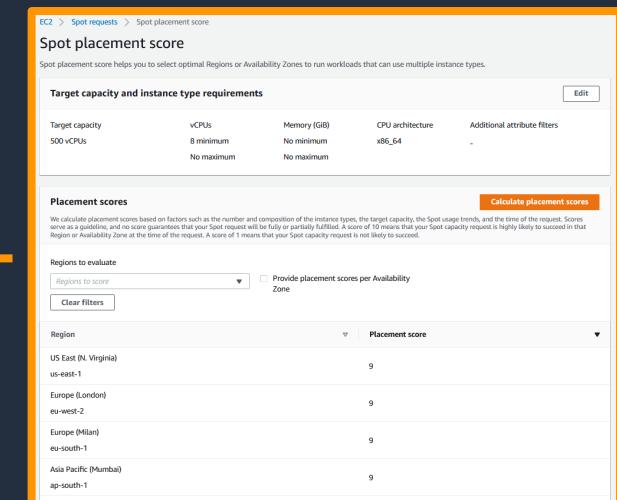
## Spot Placement Score (SPS)

Find the optimal location (Region/AZ) for your workload

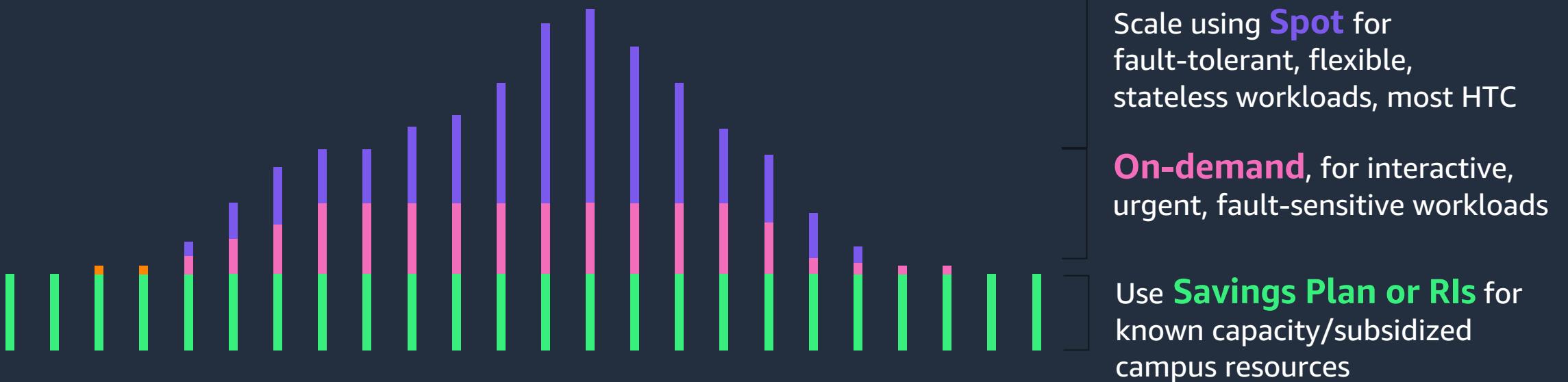
## Fault Injection Simulator (FIS)

Chaos engineering tool supporting imitation of Spot interruptions

The screenshot shows the "Instance type requirements" section of the AWS Lambda console. It includes fields for specifying instance attributes (minimum and maximum vCPUs and memory), manually adding instance types, and additional optional attributes. A purple dashed line connects this section to the "Attribute-based instance selection" section above it.



# Combine options with Organizations, EC2 Auto Scaling



# Elastic Fabric Adapter (EFA)

SRD protocol



Proving myths about latency constraints wrong



CFD

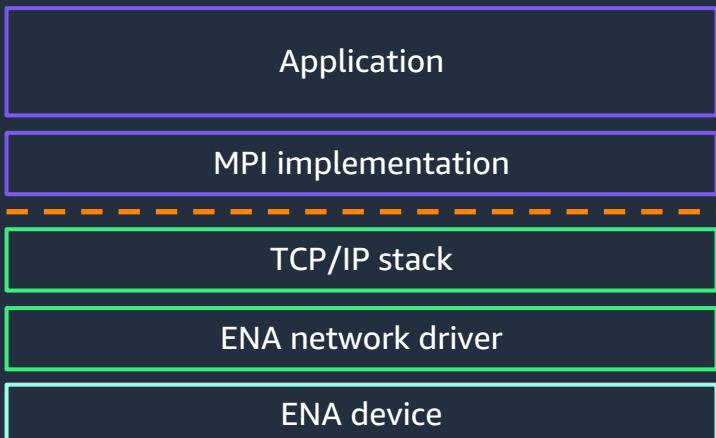


Seismic



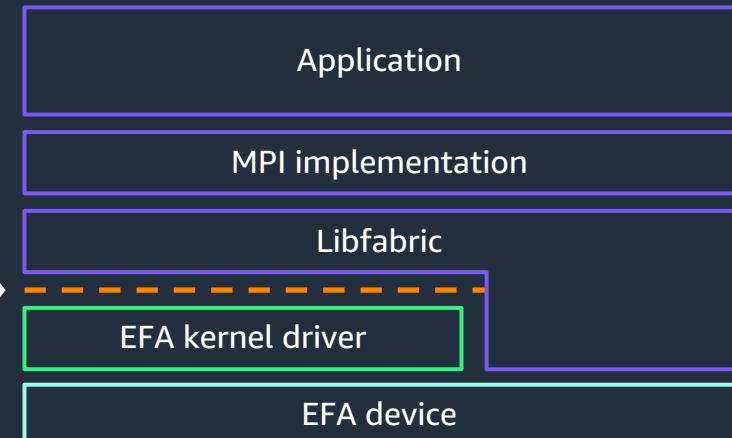
Weather modeling

Without EFA



User space

With EFA



Kernel



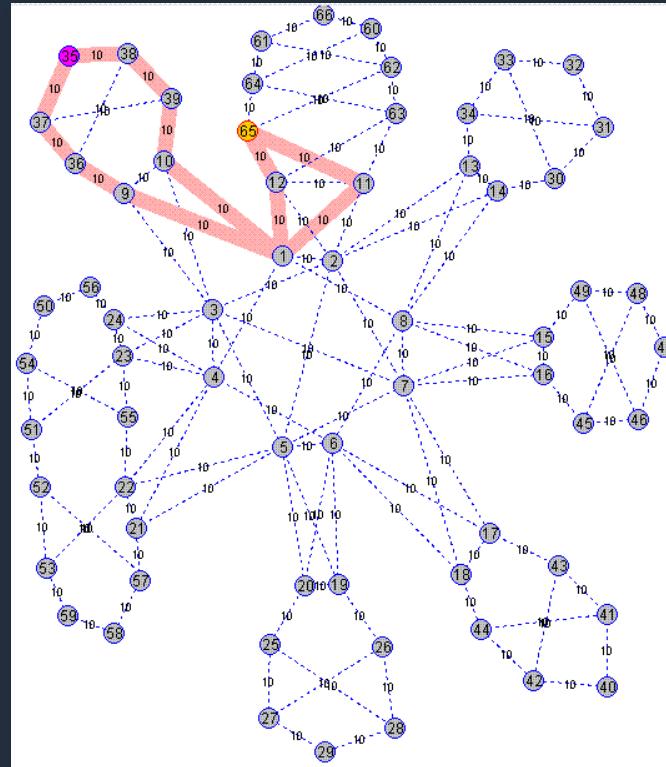


# Elastic Fabric Adapter—networks built to scale



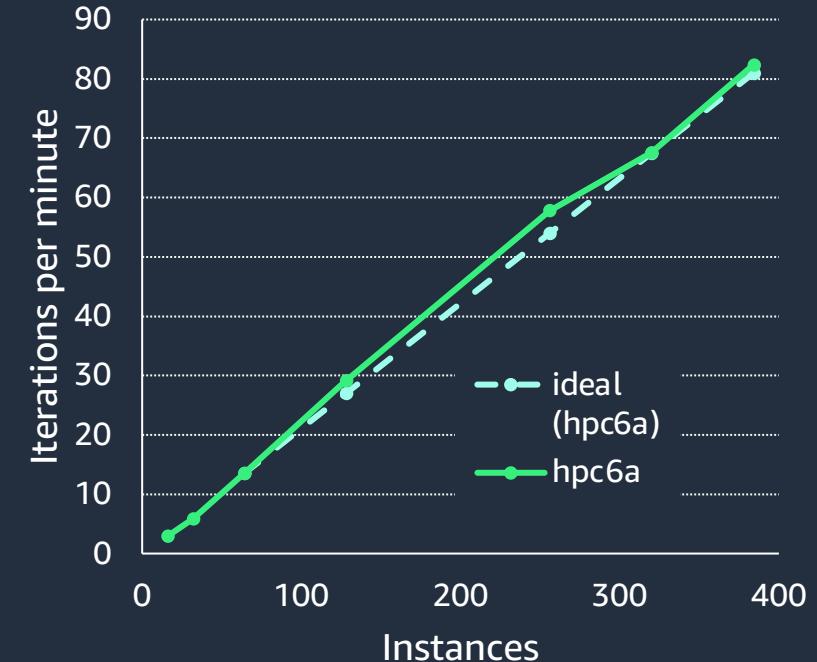
Up to  
400 Gbps  
networking  
bandwidth

- ✓ OS bypass
- ✓ GPUdirect and RDMA
- ✓ Libfabric core supports wide array of MPIs and NCCL



OCMP-enabled packet spraying  
and cloud-scale congestion control

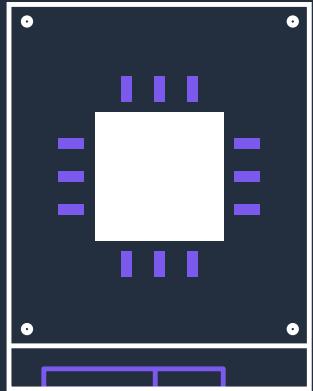
1.4B cell Siemens Simcenter STAR-CCM+ automotive CFD simulation



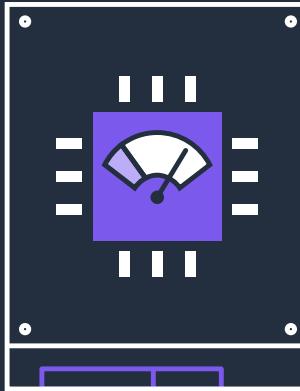
At ~40,000 cores (400 nodes), Hpc6a+EFA shows nearly 100% scaling efficiency

# Elastic Block Storage (EBS)

## SSD



**gp2 – gp3**  
General Purpose  
SSD  
\$0.08-\$0.10/GB/mo\*



**io1 – io2**  
Provisioned IOPS  
SSD  
\$0.125/GB/mo\*

## HDD



**st1**  
Throughput  
Optimized HDD  
\$0.045/GB/mo



**sc1**  
Cold  
HDD  
\$0.015/GB/mo

\* Additional provisioned throughput or IOPS charges may apply



# S3 Object Storage – a new kind of storage

Amazon S3



## S3 Standard

## S3 Intelligent-Tiering

## S3 Standard-IA

## S3 One Zone-IA

## S3 Glacier Instant Retrieval

## S3 Glacier Flexible Retrieval

## S3 Glacier Deep Archive

*Frequent*

*Access Frequency*

*Infrequent*

- Active, frequently accessed data
- Milliseconds access
- $\geq 3$  AZ
- \$0.0210/GB
- Data with changing access patterns
- Milliseconds access
- $\geq 3$  AZ
- \$0.0210 to \$0.0125/GB (\$0.004 to \$0.00099/GB Archive)
- No retrieval fees
- Monitoring fee per Obj.
- Min storage duration
- Min object size

- Infrequently accessed data
- Milliseconds access
- $\geq 3$  AZ
- \$0.0125/GB
- Retrieval fee per GB
- Min storage duration
- Min object size

- Re-creatable, less accessed data
- Milliseconds access
- 1 AZ
- \$0.0100/GB
- Retrieval fee per GB
- Min storage duration
- Min object size

- Archive data instant retrieval
- Milliseconds access
- $\geq 3$  AZ
- \$0.0040/GB
- Retrieval fee per GB
- Min storage duration
- Min object size

- Archive data
- Select minutes or hours
- $\geq 3$  AZ
- \$0.0036/GB – (\$4.10/TB)
- Retrieval fee per GB
- Min storage duration
- Min object size

- Archive data
- Select 12 or 48 hours
- $\geq 3$  AZ
- \$0.00099/GB – (\$1.01/TB)
- Retrieval fee per GB
- Min storage duration
- Min object size

# EBS and S3 – great combo



# Elastic File System (EFS) – Unlimited network storage



# Amazon FSx for Lustre

FULLY MANAGED SHARED STORAGE BUILT ON THE WORLD'S  
MOST POPULAR HIGH-PERFORMANCE FILE SYSTEM



Sub-ms latencies, **hundreds of GB/s of throughput**, millions of IOPS



**Cost-optimized file systems** with  
HDD and SSD storage options



Concurrent access for thousands of  
instances and **100,000s of cores**



**Flexible deployment options** for  
short- and longer-term workloads

Learn more: Amazon FSx for Lustre, <https://aws.amazon.com/fsx/lustre/>



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# Amazon File Cache

HIGH-SPEED CACHE FOR DATASETS STORED ANYWHERE—  
ACCELERATE AND SIMPLIFY HYBRID WORKLOADS



- **Fast**—access **cached data** at sub-millisecond latencies and hundreds of GB/s of throughput
- **Agile**—burst **compute-intensive** workloads from on premises to compute resources on AWS
- **Simple**—unify **datasets** across S3 buckets and NFS file systems into a single namespace



## Media and entertainment

VFX  
rendering/transcoding



## HPC

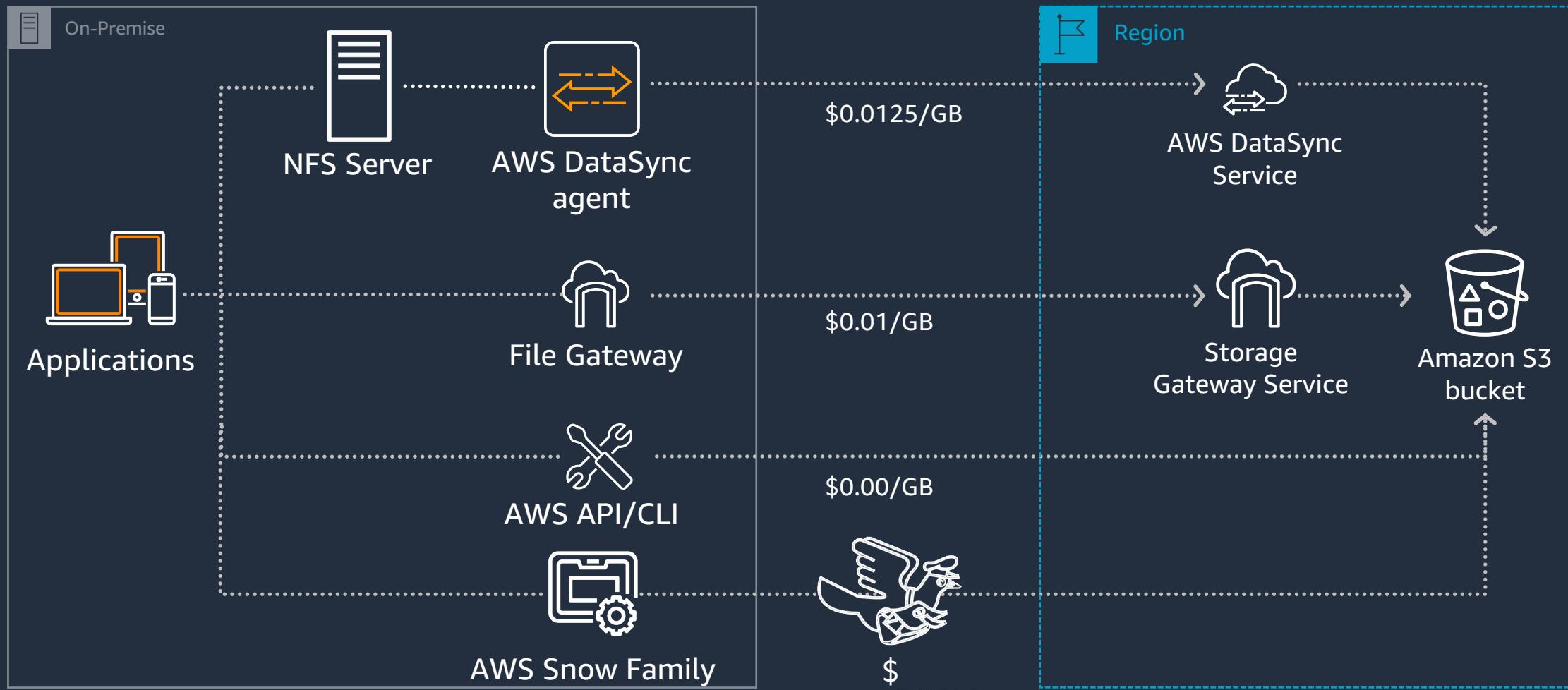
Financial services, health and life sciences,  
microprocessor design, manufacturing,  
weather forecasting, and energy



## AI/ML

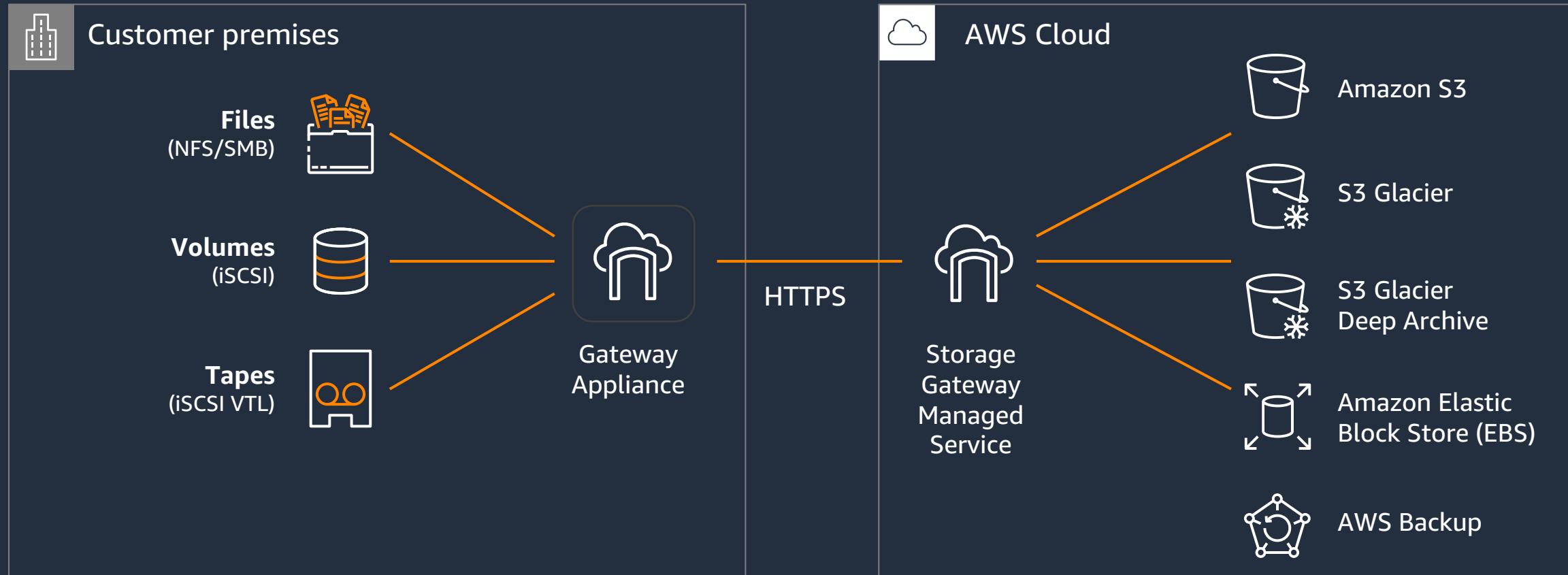
ML model training  
and large-scale analytics

# Disk/NAS to Amazon S3 Bucket



# AWS Storage Gateway

On-premises access to virtually unlimited cloud storage



Appliance Configuration: VMware, Hyper-V, EC2, Hardware  
aws

Integrated with IAM, KMS, CloudTrail,  
CloudWatch services

# Rclone

**What:** Rclone is a cross platform CLI tool enabling access to a variety of cloud storage systems, including S3, Google Drive and Box. Rclone is known as the “Swiss army knife of cloud storage” by providing familiar equivalents to commonly used CLI commands like rsync, cp, mv, mount, etc.

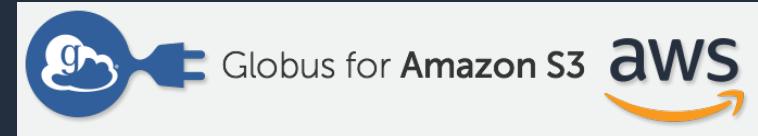
**Customer fit:** Cost conscious. Users who can use CLI tools or scripts comfortably. Users needing to move very large numbers of files (hundreds of thousands to millions.)

**Cost:** Rclone is free and Open Source (MIT). Recommend EC2 instance(s) to facilitate optimized data movement from Google Drive/Box to S3.

# Globus

A data management platform that provides secure, reliable, and efficient data transfer and sharing throughout the research lifecycle

- Web-based graphical interface is used by over 150,000 researchers around the world
- Free to use
- Subscriptions enable enhanced functionality such as data sharing and storage connectors
- Globus for Amazon S3 Connector makes transferring data into S3 simple, reliable, and efficient
- Fire and forget transfers to AWS storage



# AWS ParallelCluster – DIY clusters in AWS

One-stop shop to set up your HPC cluster



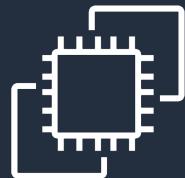
---

Integrated with AWS services you need

---



Highly-performance  
file systems



Amazon EC2  
instances

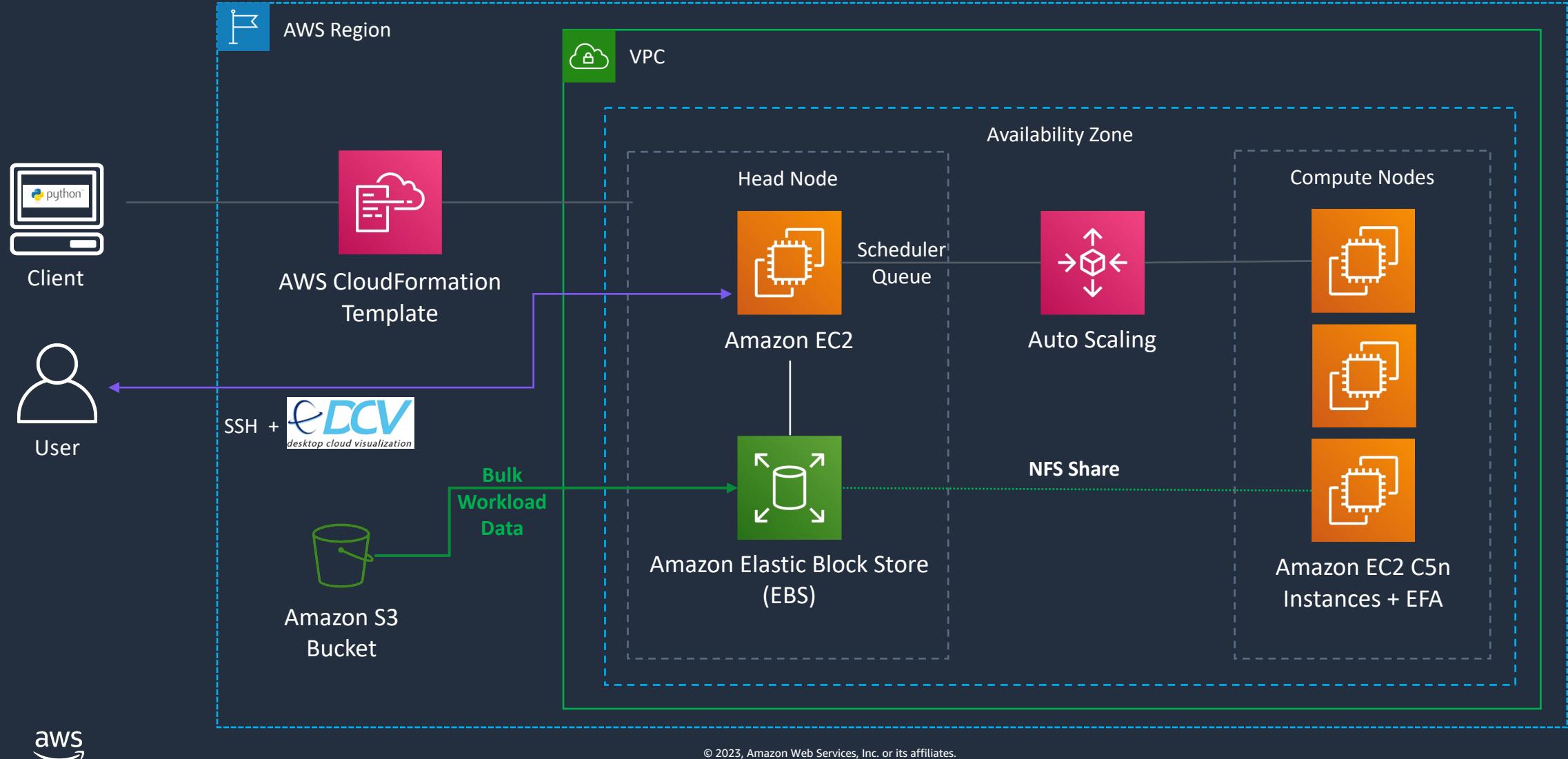


EFA



NICE DCV

# AWS ParallelCluster – generic cluster automation



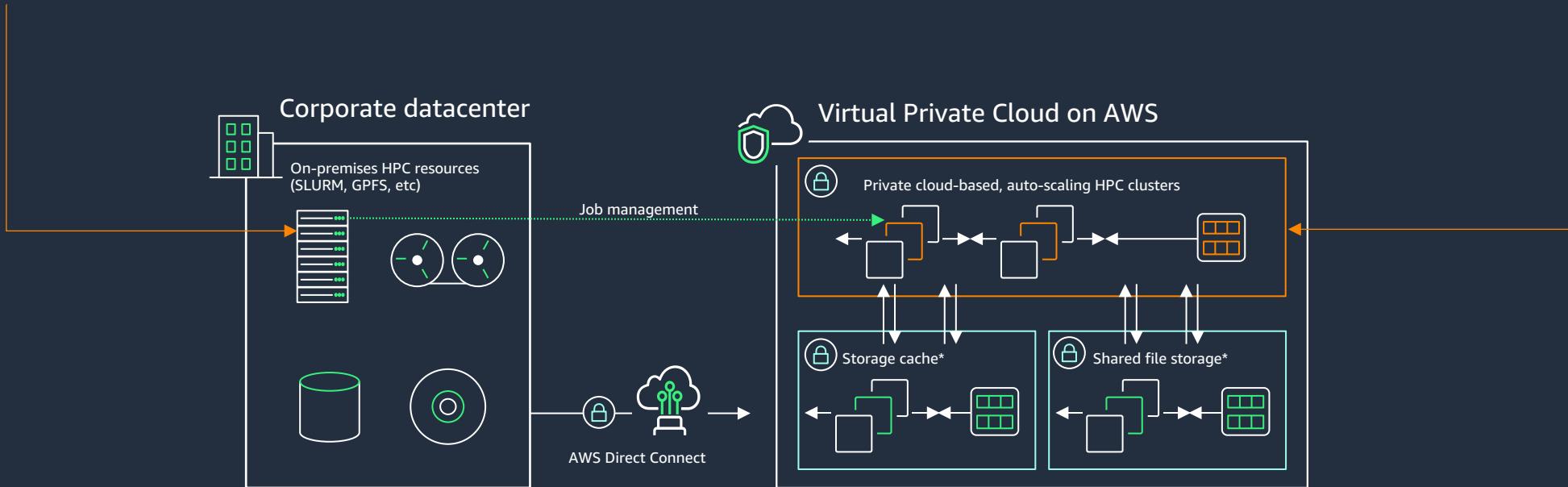
# Hybrid HPC models available

**Seamless burst** into AWS

**Same headnode** (on-premises SLURM)

**Customizable AWS partitions** (CPUs, GPUs, etc)

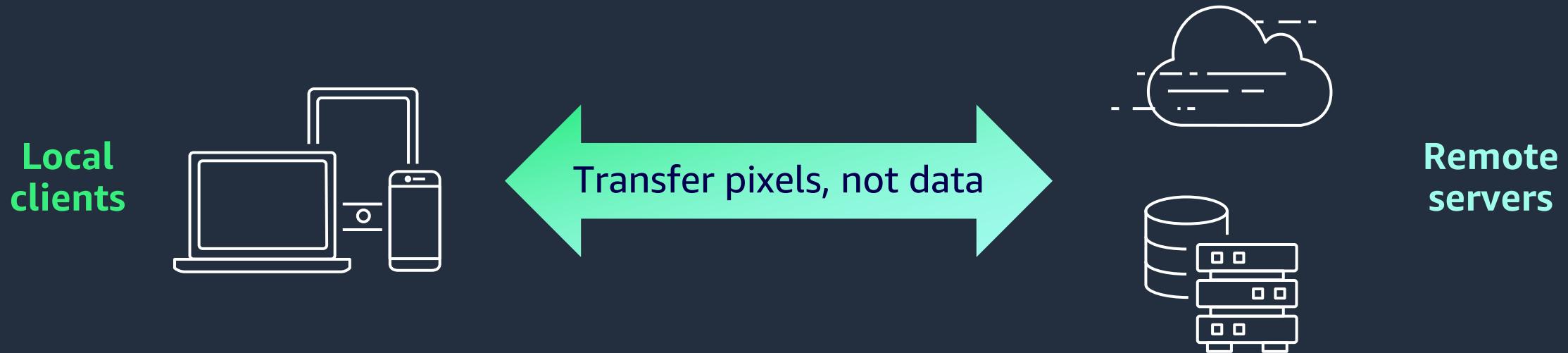
**Individual AWS accounts** for PIs, groups, labs



**Simple to onboard** through central/research IT  
**Pay as you go pricing**, on-demand/spot

# NICE DCV

**Encrypt and transport pixels to devices**



Access, manipulate, and share business-critical information,  
regardless of location, over LAN, or WAN networks

# End-user computing using DCV technology



Amazon AppStream 2.0



WorkSpaces Web



Amazon WorkSpaces

**Securely deliver desktop applications to any computer**



Centrally manage applications



Scale without infrastructure



Secure applications and data



Integrate with IT

# AWS Batch – run containers at scale



## Job scheduler

- Schedules and runs jobs asynchronously
- Manages dependencies



## Resource orchestrator

- Manages and optimizes compute resources
- Scales up/down as needed
- Utilizes the right compute resources for the job



Fully  
managed



Integrated with  
AWS services



Massive  
scalability



Optimized resource  
provisioning



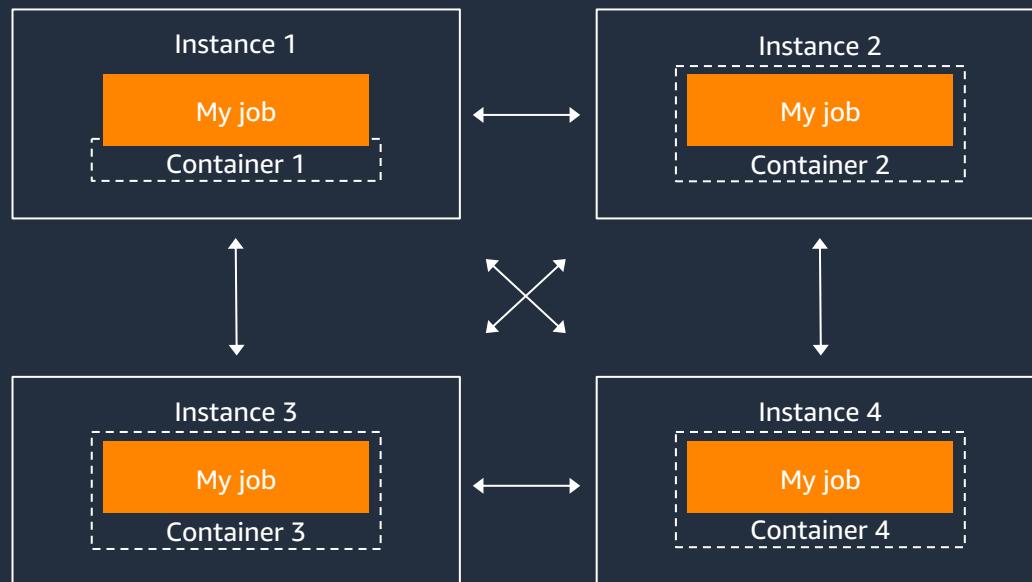
Cost  
efficient



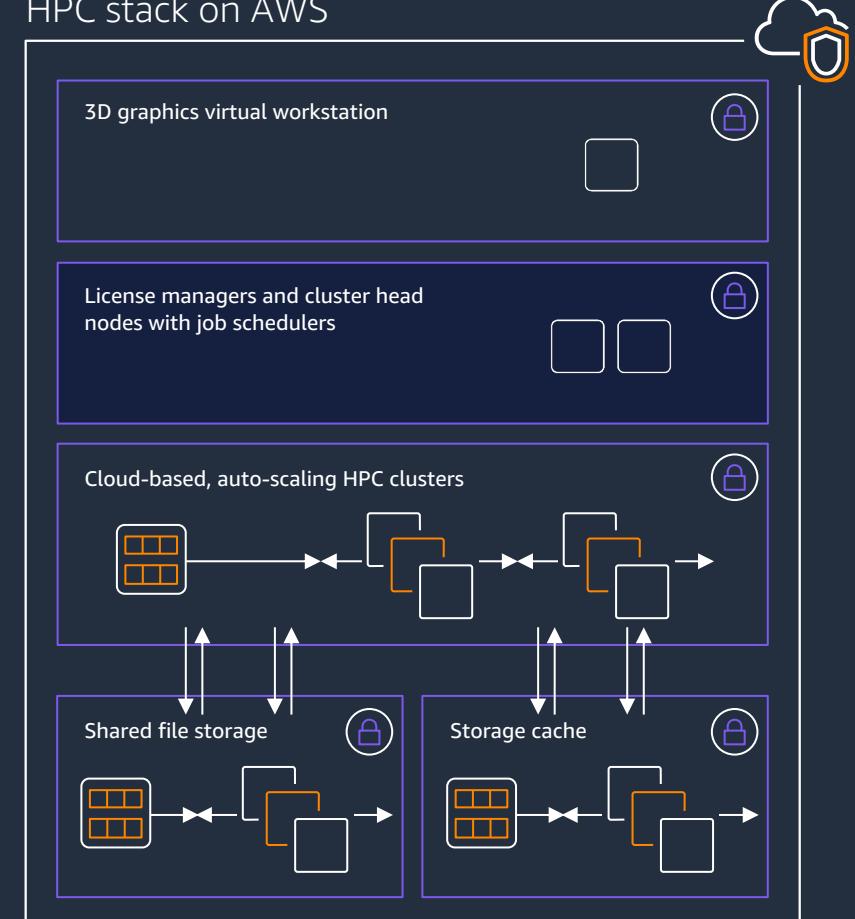
# Efficient job scheduling

## MULTI-NODE PARALLEL JOB SUPPORT ON AWS BATCH

Simplify your compute clusters and scale jobs across multiple instances with AWS Batch support for Multi-node Parallel (MNP) jobs



### HPC stack on AWS



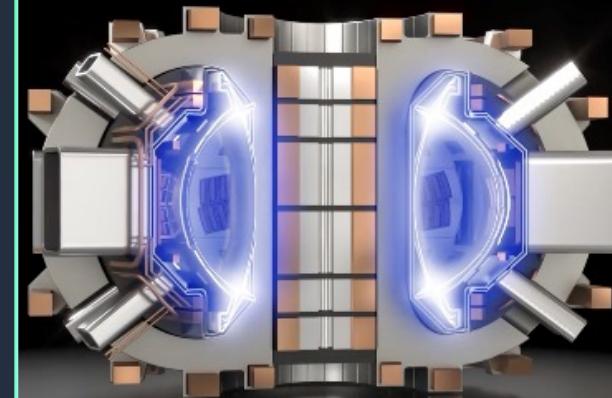
# Commonwealth Fusion Systems (CFS)

## CUSTOMER PROFILE

- Ansys Fluent, EM/Maxwell, mechanical
- **10,000+** AWS compute cores to run detailed simulations
- Almost **50%** reduction in runtime
- Reduce compute costs by more than **50%**
- Using Amazon EC2 Hpc6a.48xlarge instances to massively scale up simulations

"CFS has benefited greatly from high performance computing. The new Amazon EC2 Hpc6a has been a game changer.... We've been able to increase the speed of many simulation tasks, cut runtimes approximately in half, and reduce our computing costs by over 50%. As CFS works to bring clean, limitless commercial fusion energy to the grid, we're excited to work with AWS and their HPC team."

**Nate O'Farrell**  
Head of IT Infrastructure, Commonwealth Fusion Systems



# DTN doubles weather forecasting performance on AWS

## Challenges

Global data analytics company DTN needed to efficiently increase the frequency and accuracy of its weather forecasting models to provide more-timely insights to its customers in weather-dependent industries

## Solutions

The company is using a suite of AWS services, including Amazon EC2 Hpc6a instances, to run its high-resolution global forecast modeling workloads in the cloud and increase performance

## Results

- Increased high-resolution model frequency from two to four runs per day
- Rendered 1 hour of forecast data in under 1 minute in test scenario
- Supports faster results to customers

“Working on AWS brings agility to HPC. We can go from idea to production rapidly and scale in a way that’s beneficial to us and our customers.”

Brent Shaw

Chief Weather Architect and Director of Core Content Services, DTN



## CUSTOMER PROFILE



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INDUSTRY  
Software and internet

REGION  
United States and  
the Netherlands

---

DTN is a global data, analytics, and technology company that delivers unparalleled operational intelligence to help businesses prosper and organizations improve service delivery in the agriculture, energy, and other weather-dependent industries

# Broad HPC partner community

## Software Partners



## Consulting Partners





# Thank you!

Claudiu Farcas

[cfarcas@amazon.com](mailto:cfarcas@amazon.com)

AWS Public Sector - Education / Research

# <https://dashboard.eventengine.run>



Enter the provided  
*Event Hash*

Open AWS Console



1

Terms & Conditions:

1. By using the Event Engine 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 derivative 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 the Event Engine will comply with these terms and all applicable laws, and your access to Event Engine will immediately and automatically terminate if you do not comply with any of these terms or conditions.

Team or Event Hash (e.g. abcd-0123456789-ef)

This is the 12 or 16 digit hash that was given to you for this event or for a specific team.

✓ Invalid Hash

2

Sign in with your corporate ID

**OTP** (button highlighted with a red box)

AmazonFederate

Sign In with your social account

**Continue with Login with Amazon** (button highlighted with a yellow box)

We won't post to any of your accounts without asking first

3

### Team Dashboard

Event

AWS Console (button highlighted with a red box)

SSH Key

Event: AWS Demo

Team Name: (Team Name Not Set Yet)

Event ID: XXXXXXXXXXXX

Team ID: ZZZZZZZZZZZZ

4

### AWS Console Login

Remember to only use "us-east-1" as your region, unless otherwise directed by the event operator.

Login Link

Open AWS Console

Copy Login Link

Credentials / CLI Snippets

Mac / Linux Windows

Mac or Linux

```
export AWS_DEFAULT_REGION=us-east-1
export AWS_ACCESS_KEY_ID=[REDACTED]
export AWS_SECRET_ACCESS_KEY=[REDACTED]
export AWS_SESSION_TOKEN=[REDACTED]
```

How do I use the AWS CLI?

Checkout the AWS CLI documentation here: <https://docs.aws.amazon.com/cli/latest/userguide/cli-chap-welcome.html>

OK

# Lightsail for Research Hands-on

<https://aws.amazon.com/lightsail/research/>



# HPC Hands-on

<https://www.hpcworkshops.com/>  
Section II.a > Deploy ParallelCluster Manager (3.3.0)

Latest version (3.5.0):  
<https://docs.aws.amazon.com/parallelcluster/latest/ug/install-pcui-v3.html>

