

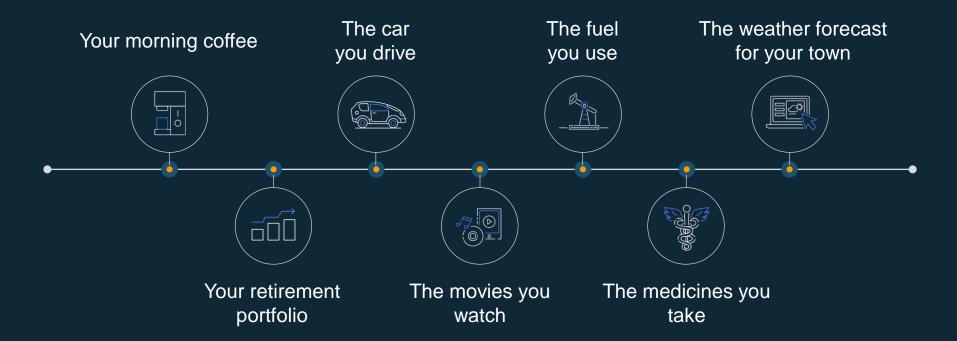
## **HPC at AWS**

Innovating without infrastructure constraints

Gilles Tourpe, <a href="mailto:gtourpe@amazon.com">gtourpe@amazon.com</a>, +33754844572

October 2020

## HPC impacts your life every day





## What if you could escape the bounds of on-premises?



Finite capacity
Queues
Engineering bottlenecks



Elasticity
Agility
Evolving ecosystem of services (e.g. AI/ML)



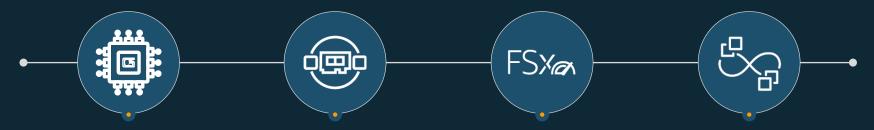
## Taking advantage of the cloud for HPC workloads



## Rethink your workflow architecture



## Continuously improving services for HPC



#### Compute

EC2 instances for every need with Intel, NVIDIA, Graviton, AMD, Inferentia and much more

#### Networking & Data Transfer

Elastic Fabric Adapter
AWS DataSync
AWS Snowball
AWS Snowmobile

#### **Data Management**

Amazon FSx for Lustre
Amazon EBS
Amazon EFS
Amazon S3
Amazon Glacier

# Orchestration, Optimization and Visualization

AWS Batch
AWS ParallelCluster
AWS EnginFrame
DCV & Appstream
AWS Spot





## Elastic Fabric Adapter

## SRD protocol



#### Proving myths about latency constraints wrong





Scale tightly coupled HPC applications on AWS



## FSXA Amazon FSx for Lustre



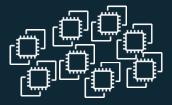
performance





100+ GiB/s throughput Millions of IOPS Consistent sub-millisecond latencies





Supports concurrent access from hundreds of thousands of cores



Conductor Technologies accelerates rendering workloads by up to 4X using Amazon FSx for Lustre





## **AWS ParallelCluster**



One-stop shop to set up your HPC Cluster

## Easy integration with AWS services







Amazon EC2 Instances



Elastic Fabric Adapter



**NICE DCV** 



**AWS Batch** 





illumına<sup>®</sup>

SCHRÖDINGER.

Tightly coupled workloads

Loosely coupled workloads

Accelerated computing







Visualization

AI/ML

High-volume data analytics





## INEOS TEAM UK

INEOS TEAM UK accelerates boat design for America's Cup using AWS

"Working with AWS has given us access to more and faster computational resources, which has proven crucial in developing the fastest race boat possible. It has helped the team push ahead as we continue to design and develop our race boat for the America's Cup. "

Sir Ben Ainslie Team Principal and Skipper



#### Formula 1 / AWS Partnership – All about Data. Large-Scale CFD Simulations



- Simulation time reduced from 60hrs to 18hrs thanks to AWS.
- Two car turbulence simulations increased from 1 to 5 on AWS
- 192 cores to 1440 cores (C5n with EFA + AWS ParallelCluster)
- For more on how Formula 1 is using AWS, visit: aws.com/f1

"This project with AWS was one of the most revolutionary in the history of Formula 1 aerodynamics "

**Pat Symonds**, Chief Technical Officer of Formula 1









Toyota Research Institute chooses FSx for Lustre to reduce object recognition machine learning training times

"We needed a parallel file system for our ML training data sets and chose Amazon FSx for Lustre... the integration with AWS services, including S3, also made it the preferred option for our high performance file storage."

David Fluck, Software Engineer Toyota Research Institute



## Standard Chartered cuts Risk Grid Costs 60%



### **Re-Imagining the HPC Workflow**

"Grid computing is an ideal workload for the cloud, so working with AWS technology was the easy part."

Richard Davis
Global Head of Technology Services, Standard Chartered

Innovative Cloud HPC architecture with Amazon Spot, Lambda, & RDS



## FactSet migrates its Real-Time Ticker Plant to AWS

"Moving a full ticker plant onto the cloud is the holy grail of market data engineers. Many people thought it would be impossible. ... AWS provides a stable and secure environment for processing major exchange feeds. We are confident that this groundbreaking project will help us drive greater speed and efficiency to accelerate our clients' digital transformations."



Gene Fernandez, Chief Product and Technology Officer, FactSet.

#### Challenge

FactSet's Ticker Plant, ingests and delivers live market data from exchanges globally

#### **Solution**

The company will rely on AWS services and AWS EC2 instances to build their **Real-Time Ticker Plant** service on AWS.

#### **Benefits**

- Increased scalability of the Service
- Increased overall performance
- First Global Ticker Plant of this kind on the Cloud



#### AstraZeneca raising the bar running their Genome sequencing pipeline on AWS

- Goal: To analyze 2M genomes by 2026. Scale and Orchestration to build the fastest and most efficient sequence data pipeline in the industry.
- Decreased processing time by 2400% from 20 days to 20 hours for 20,000 samples
- Providing scientists with advanced access to the clinical effects of natural mutations in humans that mimic drug inhibition/suppression for the majority of human genes
- FPGA instances for compute and Step Functions, Lambda, S3, SQS and AWS Batch.

"Building our bespoke analysis pipeline on AWS with the support of AWS Professional Services has enabled us to achieve acceleration of key objectives towards the analysis of up to 2 million genomes (AstraZeneca's Genomics Initiative)."



Slavé Petrovski

PhD Vice President and Head of Genome Analytics and Bioinformatics, Discovery Sciences, R&D



#### Lyft increases simulation capacity, lowers costs using Amazon EC2 Spot Instances

#### Challenge

Rideshare company Lyft runs millions of compute-intensive simulations each year to improve the performance and safety of its self-driving system requiring computing power that could scale up and down at an affordable price.

#### **Solution**

The company significantly increased its AV simulation testing while reducing the corresponding computing costs by two-thirds with Amazon EC2 Spot Instances and Amazon EKS.

#### **Benefits**

- Reduced compute costs by two-thirds
- Scaled up computing capacity significantly
- Increased velocity of development for AVs



Company: Lyft

Industry: Transportation & Logistics

**Country: United States** 

#### **About**

Lyft, one of the largest transportation networks in the United States and Canada, is on a mission: improve people's lives with the world's best transportation. It provides shared rides, electric scooters, bikeshare systems, and public transit partnerships.

"About 77% of our computing fleet is now on Amazon EC2 Spot Instances. We were able to scale up our computing capacity significantly while reducing the overall cost of operation."

Timothy Perrett, Level 5 senior staff engineer, Lyft



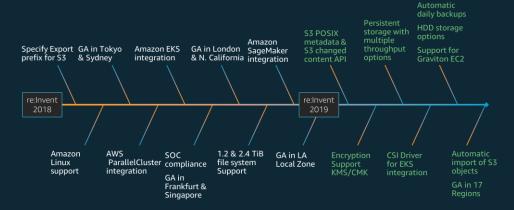
## The pace for innovation never slows

#### **Batch**

- Graviton2, AMD, and Inferentia support
- Increased capability for high-throughput workloads
- Custom Log Drivers (Splunk, Fluentd),
- New console: visibility improvements, sorting, and filtering
- Custom Retry capabilities

#### ParallelCluster 2.9

- Multiple Job Queues
- Multiple instance types per queue
- Support for Graviton2
- DCV for visualization
- FSx for Luste Integration
- Cloudwatch Logs
- Amazon Linux 2, Ubuntu 18 support



FSx for Lustre Innovations



## Interesting public resources

https://aws.amazon.com/fr/hpc/
https://pages.awscloud.com/hpc-cae-credit-code-2020.html

https://d1.awsstatic.com/whitepapers/benchmarking-aws-and-hpcservices.pdf?did=wp\_card&trk=wp\_card

https://aws.amazon.com/blogs/opensource/category/compute/aws-parallel-cluster/https://aws.amazon.com/blogs/storage/category/storage/amazon-fsx-lustre/https://aws.amazon.com/blogs/compute/category/compute/aws-batch/https://aws.amazon.com/blogs/compute/category/compute/high-performance-computing/





# Thank You!

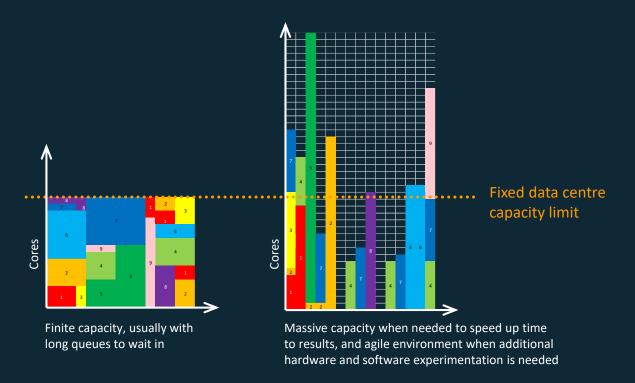




# **High Performance Computing on AWS**

Innovating without infrastructure constraints

# We think the metric for success for any business should be time-to-results



"For every \$1 spent on HPC, businesses see \$463 in incremental revenues and \$44 in incremental profit."

-Hyperion Research, 2018



## Because, a TCO analysis never tells the whole story

#### Lost productivity & longer time to results

72.8%

of organizations that use HPC reported delayed or cancelled HPC jobs\*



#### Lost innovation

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



#### **Outdated technology**

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



#### **Technical debt**

Adapting newer algorithms to meet the requirements of an existing infrastructure = delays, and belowpar performance.



<sup>\*</sup> Source: Hyperion Research, 2018

## HPC on AWS is a fundamental rethink of what is possible

to

## From worrying about



Capex Capacity Technology

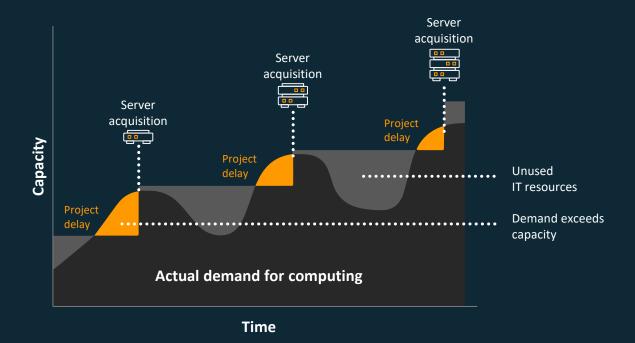


Focusing on innovation



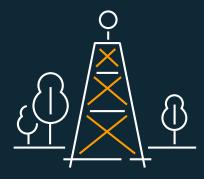
## Matching demand to capacity is challenging

Attempting to match variable computing demand to static on-premise compute grids is extremely difficult, and adding capacity is time- and capital-intensive





## And the choices poor



**Optimize for availability** 

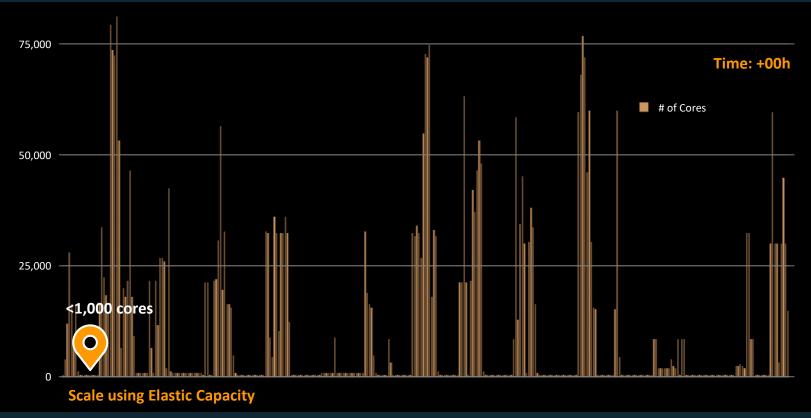
Usage remains low which drives up costs



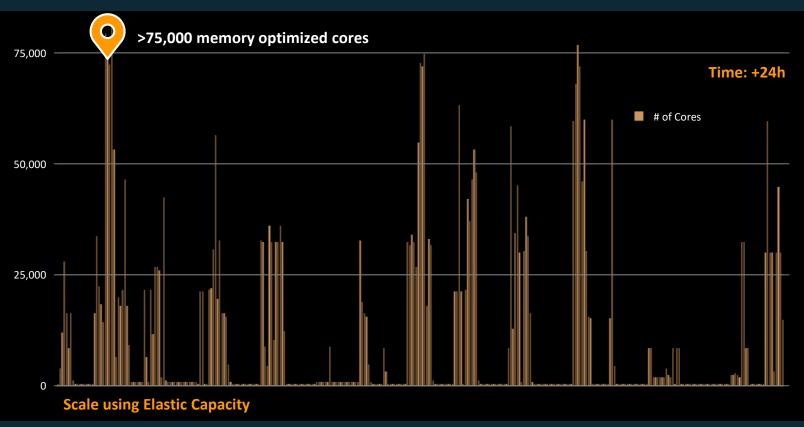
**Optimize for cost** 

Utilization is high but users may wait a long time to access the system

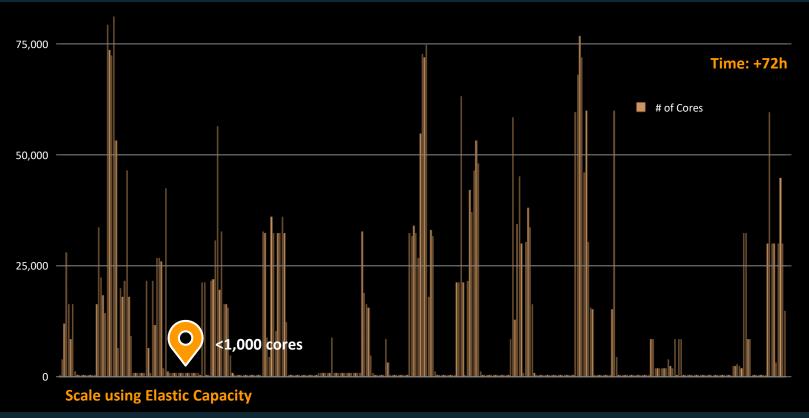




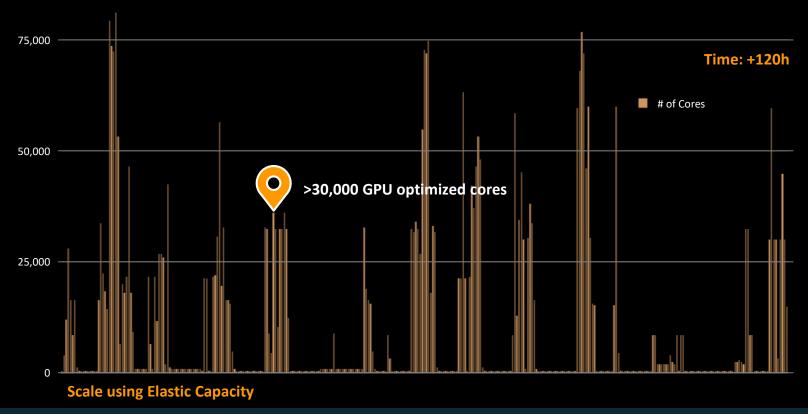














### HPC on AWS

## Accessible and on-demand elastic compute power

What if you could add thousands of cores of your choice to your HPC infrastructure as you needed them, remove them when you are done, and only pay what you used?



How would that kind of additional compute power improve your time-to-results?



## Why HPC on AWS?

Virtually unlimited infrastructure enabling scaling and agility not attainable on-premises

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

Flexible configuration options quickly iterate resource selection and ensure cost optimization



**Better ROI** 

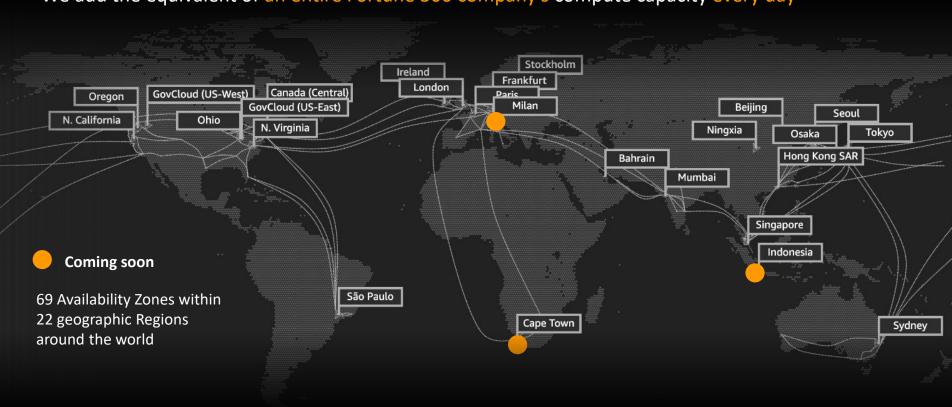


Faster time to results



## Global Infrastructure

We add the equivalent of an entire Fortune 500 company's compute capacity every day



## High Performance Computing on AWS

AWS & Partner service options for every layer of the HPC stack





## AWS Services to get started with HPC on AWS

Amazon CloudWatch				
Data management & data transfer	Compute & networking	Storage	Automation & orchestration	Visualization
AWS DataSync AWS Snowball AWS Snowmobile AWS DirectConnect	Amazon EC2 instances (CPU, GPU, FPGA)  Amazon EC2 Spot  AWS Auto Scaling  Placement groups  Enhanced networking  Elastic Fabric Adapter	Amazon EBS with provisioned IOPS Amazon FSx for Lustre Amazon EFS Amazon S3	AWS Batch AWS ParallelCluster NICE EnginFrame	NICE DCV Amazon AppStream 2.0

**Amazon IAM (Identity and Access Management)** 

**AWS Budgets** 



## Broad HPC partner community

#### **Application partners**













DN/\nexus



**illumına**°



Infrastructure partners









Technology partners





Consulting partners

**CADFEM** 











## Infrastructure is code. Not a 5-yearly refresh

```
↑ bouffler — -bash — 80×24
Last login: Thu May 30 12:57:28 on ttys000
(base) ~ [1] $
```

**Iteratively** decide on the best CPU, GPU, memory or I/O architecture for your workload

Test multiple options in parallel rather than sequentially

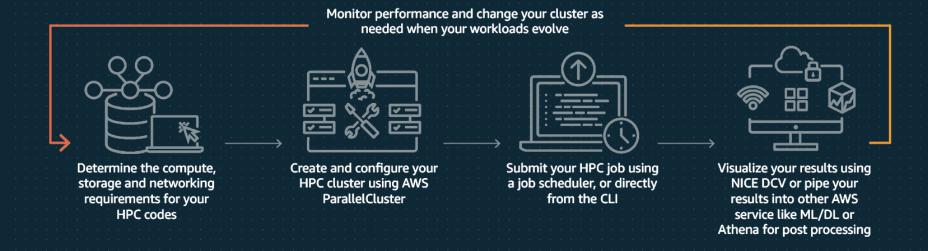
Dispose of what you don't need

Make CI/CD part of your HPC practice

Link to tutorial <INSERT>

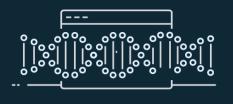


### Simple steps to get started





#### HPC workloads across industries



**Life Sciences** 



**Financial Services** 



Oil & Gas



**Design & Engineering** 



**Climate & Geosciences** 



**Autonomous Vehicles** 



#### HPC workloads across industries







**Life Sciences** 

**Financial Services** 

Oil & Gas







**Design & Engineering** 

**Climate & Geosciences** 

**Autonomous Vehicles** 



### HPC workloads with different compute and throughput characteristics



**Tightly-coupled workloads** 



**Loosely-coupled workloads** 



**Accelerated computing** 



Visualization



AI/ML



High volume data analytics



### HPC workloads with different compute and throughput characteristics

**VOLKSWAGEN** 

GROUP

**Tightly-coupled workloads** 

**illumına**°

**Loosely-coupled workloads** 

SCHRÖDINGER.

**Accelerated computing** 



Visualization



AI/ML



High volume data analytics



### **HPC on AWS: solution components**



### High Performance Computing (HPC) on AWS

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



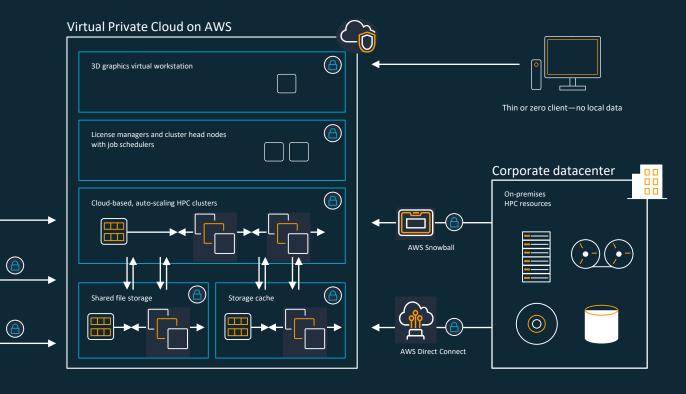
Machine learning and analytics



Amazon S3 and Amazon Glacier



Third-party IP providers and collaborators





### Broadest and deepest platform choice

# Categories General purpose Burstable Compute intensive Memory intensive Storage (High I/O)



Dense storage

**Graphics intensive** 

#### **Capabilities** NEW Choice of processor (AWS, Intel, AMD) Fast processors (up to 4.0 GHz) High memory footprint (up to 12 TiB) Instance storage (HDD and NVMe) Accelerated computing (GPUs and FPGA) Networking (up to 100 Gbps) Bare Metal Size (Nano to 32xlarge)

#### **Options**

Elastic Block Store

Elastic Graphics

Elastic Inference



instance types

for virtually every workload and business need

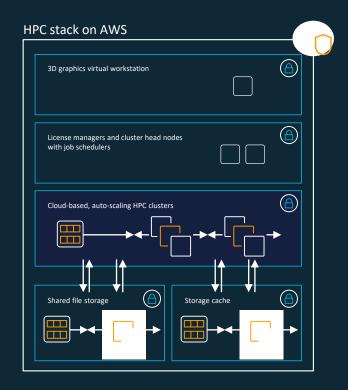


### High bandwidth compute instances: C5n

#### 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

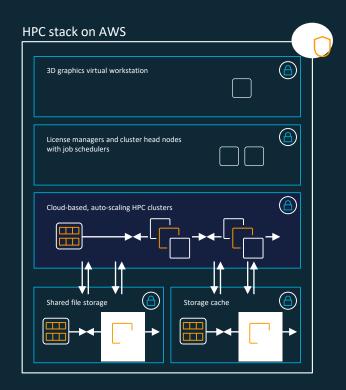




### High bandwidth compute instances: P3dn

#### Optimized for distributed ML training

- One of the most powerful GPU instance available in the cloud
- Distributed machine learning training across multiple GPU instances
- 100 Gbps of networking throughput
- Based on NVIDIA's latest GPU Tesla V100 with 32GB of memory each
- The largest Amazon Elastic Compute Cloud (Amazon EC2)
   P3 instance size available



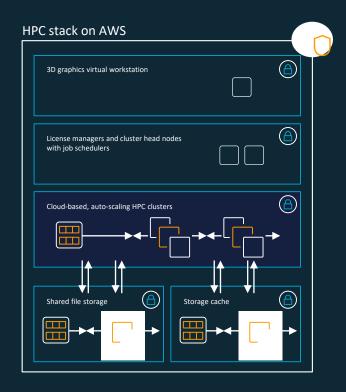


### High clock speed compute instances: Z1d

#### Up to 4 GHz sustained, all-turbo performance

- Z1d instances are optimized for memory-intensive, compute-intensive applications
- Custom Intel Xeon Scalable processor
- Up to 4 GHz sustained, all-turbo performance
- Up to 385GiB DDR4 memory
- Enhanced networking, up to 25 GB throughput

Featuring Intel Xeon Scalable (Skylake) processor





### Elastic Fabric Adapter (EFA)

Scale tightly-coupled HPC applications on AWS

C5n

P3dn

i3en







### **EFA**

Elastic Fabric Adapter, best for large HPC workloads

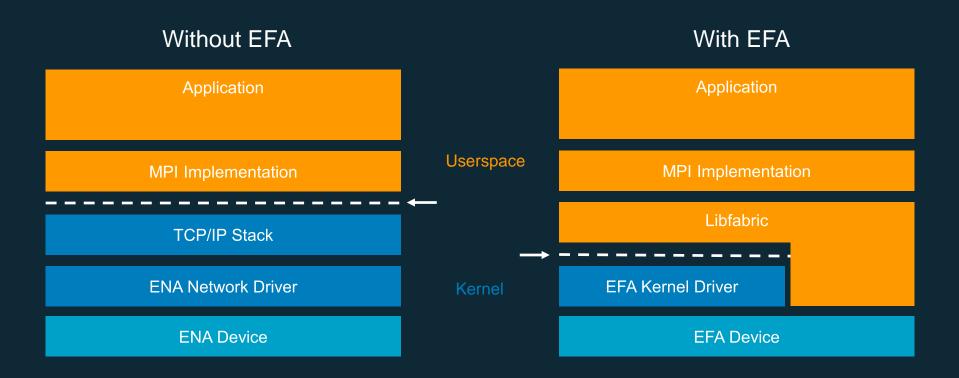
Scale tightly-coupled HPC and ML workloads

100 Gbps network bandwidth

< 15 micro-seconds network latencies

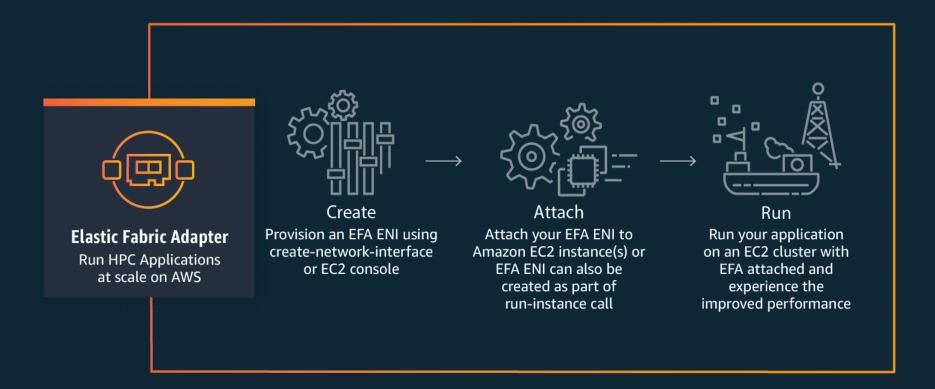


### HPC software stack in Amazon EC2



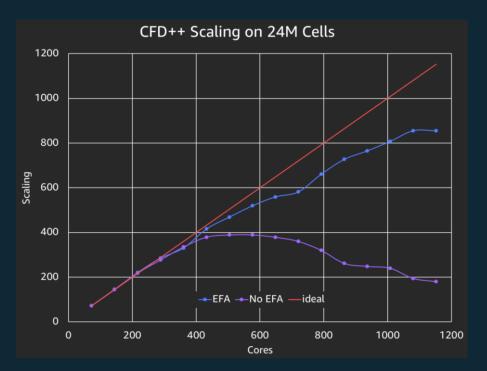


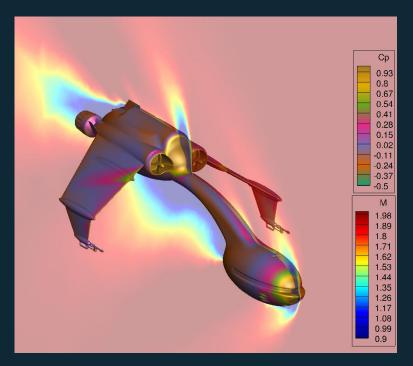
### Getting started with EFA on AWS





### What can EFA do?





Thanks to Metacomp Technologies and the Klingon Empire.



### Enhanced Network for HPC and machine learning

Up to 100 Gbps network bandwidth

C5n

Most elastic and scalable HPC network



Custom Intel® Xeon® Scalable processor

P3dn

Fastest machine learning training in the cloud



NVIDIA V100 Tensor Core GPUs



Elastic Fabric Adapter for HPC
Best for scaling large HPC and ML workloads



### Comprehensive portfolio of high performance storage options

**Block storage** 



**Amazon EBS** 

Elastic, high performance block storage at any scale

File storage



**Amazon EFS** 

Petabyte-scale, elastic file storage sharable across applications, instances and servers

Object storage



**Amazon S3** 

Low cost, highly scalable cloud storage with 99.999999999 durability



### Fully managed high performance shared file system: Amazon FSx for Lustre

#### Massively scalable performance

100+ GiB/s throughput

Millions of IOPS

Consistent low latencies



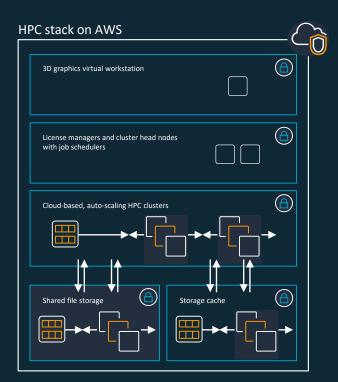
High performing



Parallel distributed file system



Tune complex performance parameters





### High and scalable performance



performance

Parallel File System



SSD-based





100+ GiB/s throughput
Millions of IOPS
Consistent sub-millisecond latencies



Supports concurrent access from hundreds of thousands of cores

Each terabyte (TB) of storage provides 200 MB/second of file system throughput and ~5,000 IOPS



### File system throughput and IOPS scale linearly with storage capacity



Each TB of storage provides 200 MB/s of baseline throughput, and up to 12x burst throughput

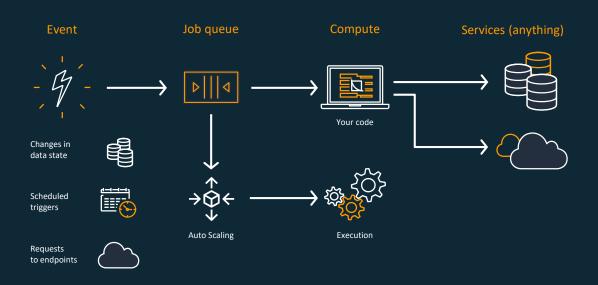
File systems can scale to hundreds of GB/s and millions of IOPS

Capacity	Baseline throughput	Burst throughput
1TB	200 MB/s	up to 2.4 GB/s
10TB	2 GB/s	up to 24 GB/s
50TB	10 GB/s	up to 120 GB/s
100ТВ	20 GB/s	up to 240 GB/s
1PB	200 GB/s	at least 240 GB/s



#### **AWS Batch**

AWS Batch dynamically provisions resources, plans, schedules, and executes No additional components to install

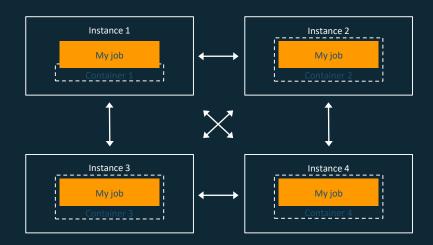


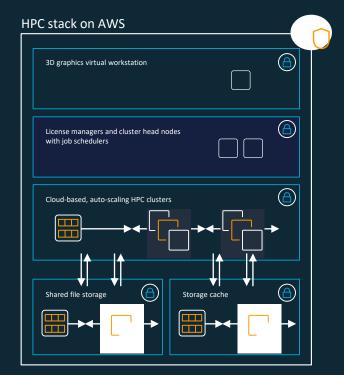




### Efficient job scheduling: Multi-node parallel job support on AWS Batch

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







### Easy cluster management: AWS ParallelCluster



Simplifies deployment of HPC in the cloud, including integrating with popular HPC schedulers

Integrated with AWS Batch, Amazon FSx for Lustre and Elastic Fabric Adapter

Link to tutorial <INSERT>



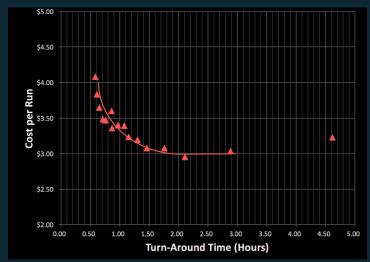
### Simplifying capacity and cost optimization

Scale using Spot, On-Demand, or both

Use Reserved Instances for known/steady-state workloads

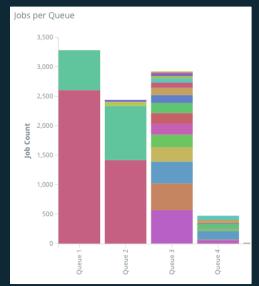


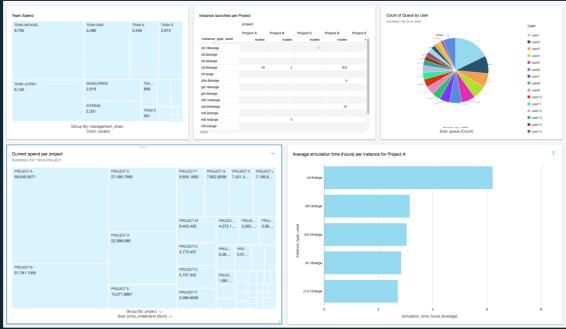
Evaluate the trade-off of time to solution vs. cost for scaling





### Use AWS services to manage, analyze, and visualize operational metrics







### Track your spend with AWS Cost Explorer

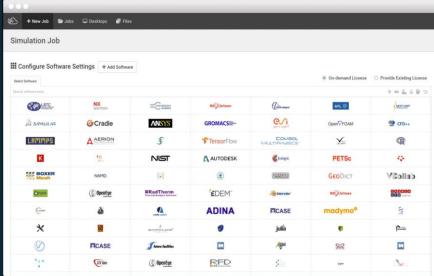




### Multiple partner options to get started

If DIY HPC clusters are not your thing, explore our rich partner community







### Compliance programs

Global















SOC 2





Europe









Asia Pacific











United States































### AWS is the first choice for highly regulated organizations

"

We can be far more secure in the cloud and achieve a higher level of assurance at a much lower cost, in terms of effort and dollars invested. We determined that security in AWS is superior to our on-premises data center across several dimensions, including patching, encryption, auditing and logging, entitlements, and compliance.



- John Brady, CISO, FINRA



Over 50 global compliance certifications and accreditations



AWS industry-leading security teams: 24/7, 365 days a year



Security infrastructure built to satisfy military, global banks, and other high-sensitivity organizations



Security enhancements from 1M+ customer experiences



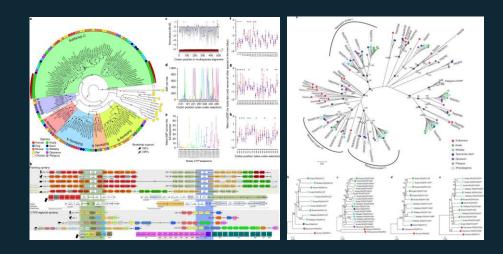
## Driving business outcomes and making a difference





### Complete sequencing of 3.24 billion base pairs

3 million core-hours of Amazon EC2 Spot capacity



https://www.nature.com/articles/s41588-018-0153-5





### Helping financial institutions model investment risks

Run risk models

### 4,000 times faster

In hours, instead of months

Manage 50X the number of securities





### Running HPC applications at extreme scale

Accelerating time to innovation



Over 2.3 million simulation jobs on a single HPC cluster of 1 million vCPUs

—built using Amazon EC2 Spot Instances

Time to results: 20 days → 8 hours

"Storage technology is amazingly complex and we're constantly pushing the limits of physics and engineering to deliver next-generation capacities and technical innovation. This successful collaboration with AWS shows the extreme scale, power and agility of cloud-based HPC to help us run complex simulations for future storage architecture analysis and materials science explorations. Using AWS to easily shrink simulation time from 20 days to 8 hours allows Western Digital R&D teams to explore new designs and innovations at a pace un-imaginable just a short time ago." —Steve Phillpott, CIO, Western Digital





#### **HPC on AWS**

Flexible configuration and virtually unlimited scalability to grow and shrink your infrastructure as your HPC workloads dictate, not the other way around

