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EMEA HEALTHCARE & LIFE SCIENCES - VIRTUAL

AWS HCLS Workshops

Join our series of free one-day technical workshops on compliance, genomics, machine learning, manufacturing, sustainability, and more. Led by AWS industry experts.

June 27 – July 18 2023

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Running High-Performance Computing on AWS

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Amazon Web Services

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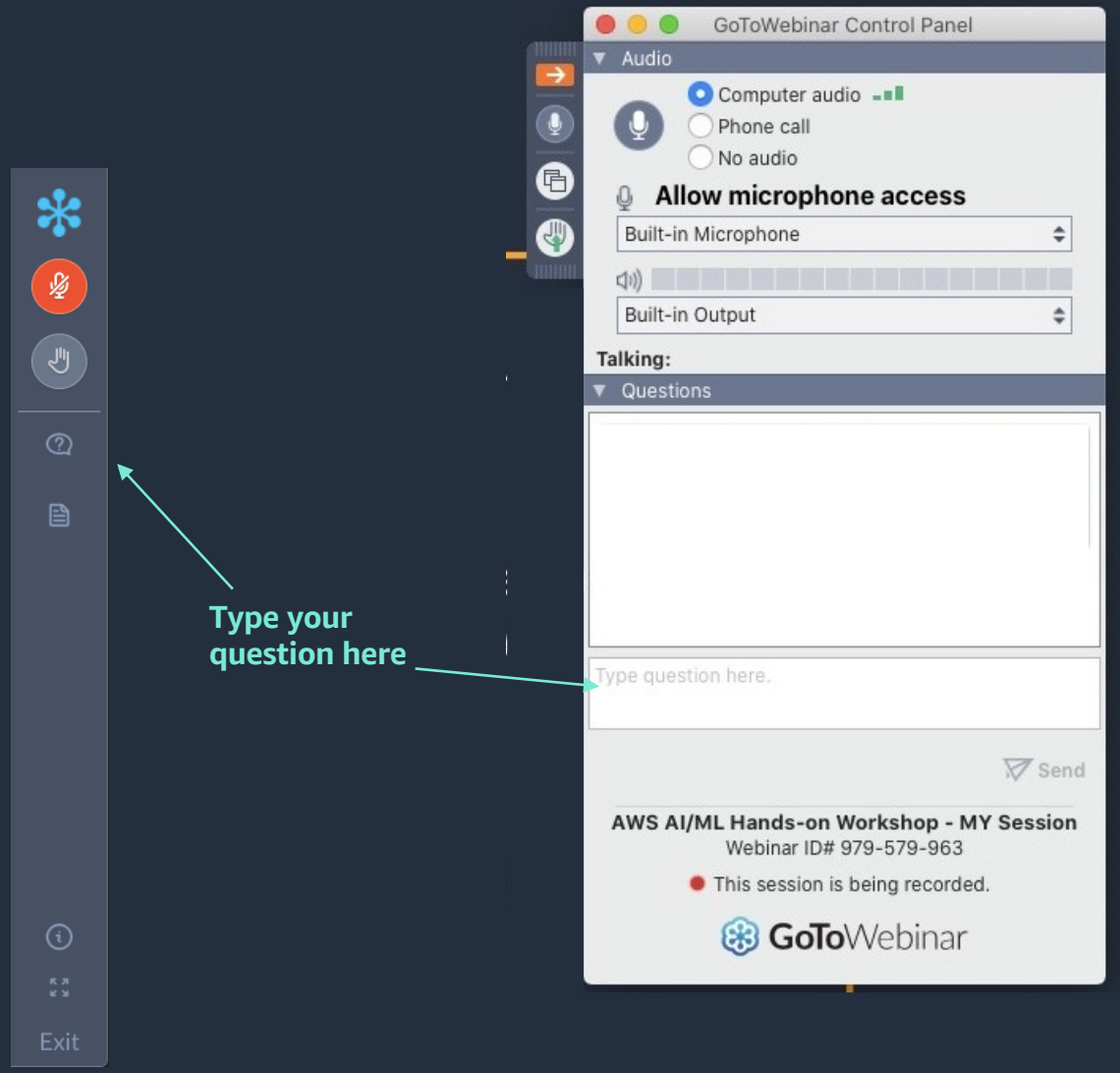
Solutions Architect
Amazon Web Services

Matt Pawelczyk
Associate Solutions Architect
Amazon Web Services

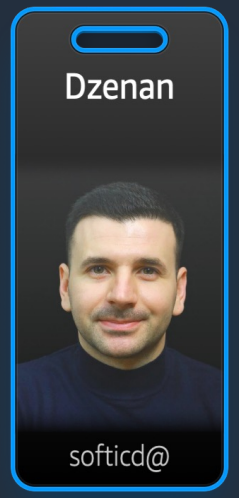
Questions & Answers

If you have any questions or encounter issues during the workshop, our support team is online.

You can submit your query in the GoToWebinar Questions function. To submit questions, select
“Send”



Your presenters today



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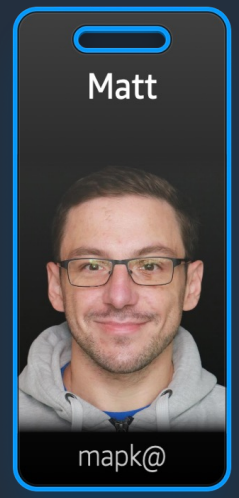

Matt Pawelczyk

mapk@amazon.de

Agenda

- 13:05 – 13:35 High Performance and Accelerated Computing on AWS
- 13:35 – 14:00 Account Setup and Coffee Break
- 14:00 – 14:45 AWS Batch and Implementation for Protein Folding
- 14:45 – 16:45 Hands-on Workshop: Molecular Dynamics with GROMACS
- 16:45 – 17:00 Q&A Session

Workshop materials and instructions

- https://catalog.workshops.aws/gromacs-on-aws-parallelcluster/en-US

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https://aws-experience.com/

- June 27th: AWS Cloud Fundamentals
- June 28th: Genomic Data Analysis with Amazon Omics
- July 4th: Machine Learning
- July 5th: AWS for Pharma Manufacturing
- July 6th: Security, Encryption & Data Protection Immersion Day
- July 11th: Sustainability
- **July 13th: High-performance computing**
- July 18th: Compliance in the Cloud

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Please complete the workshop survey

https://s12d.com/6UMF89g1

High Performance and Accelerated Computing on AWS

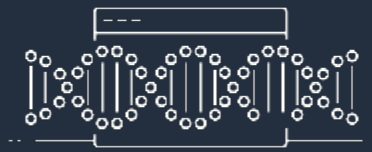
HPC is all around us

Build designs faster with computational fluid dynamics (CFD) simulations

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

Process complex workloads and analyze massive data pipelines to further research

Fast-track drug discovery and structure-based drug design



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

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Defining HPC – Example Use Cases

Clustered (Tightly coupled)

Data Light

Minimal requirements for high performance storage

- Fluid dynamics
- Weather forecasting

- Clinical trial simulations
- Astrophysics
- Deep learning

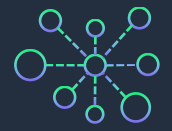
Data Heavy

Benefits from access to high performance storage

- Molecular modeling
- Risk simulations

- Genomics
- Animation and VFX

Distributed / Grid (Loosely coupled)



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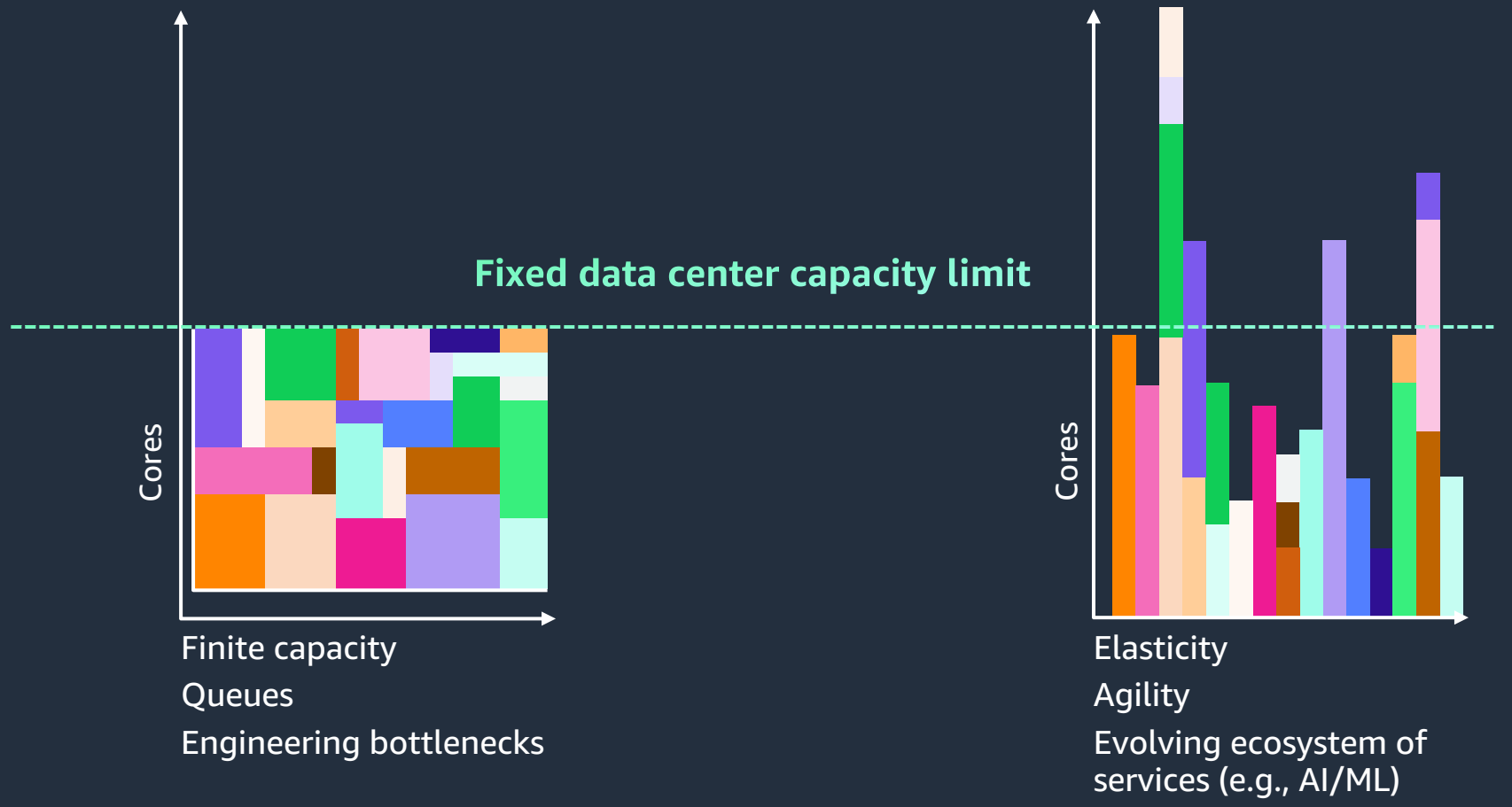
What if you could escape the bounds of on-premises?



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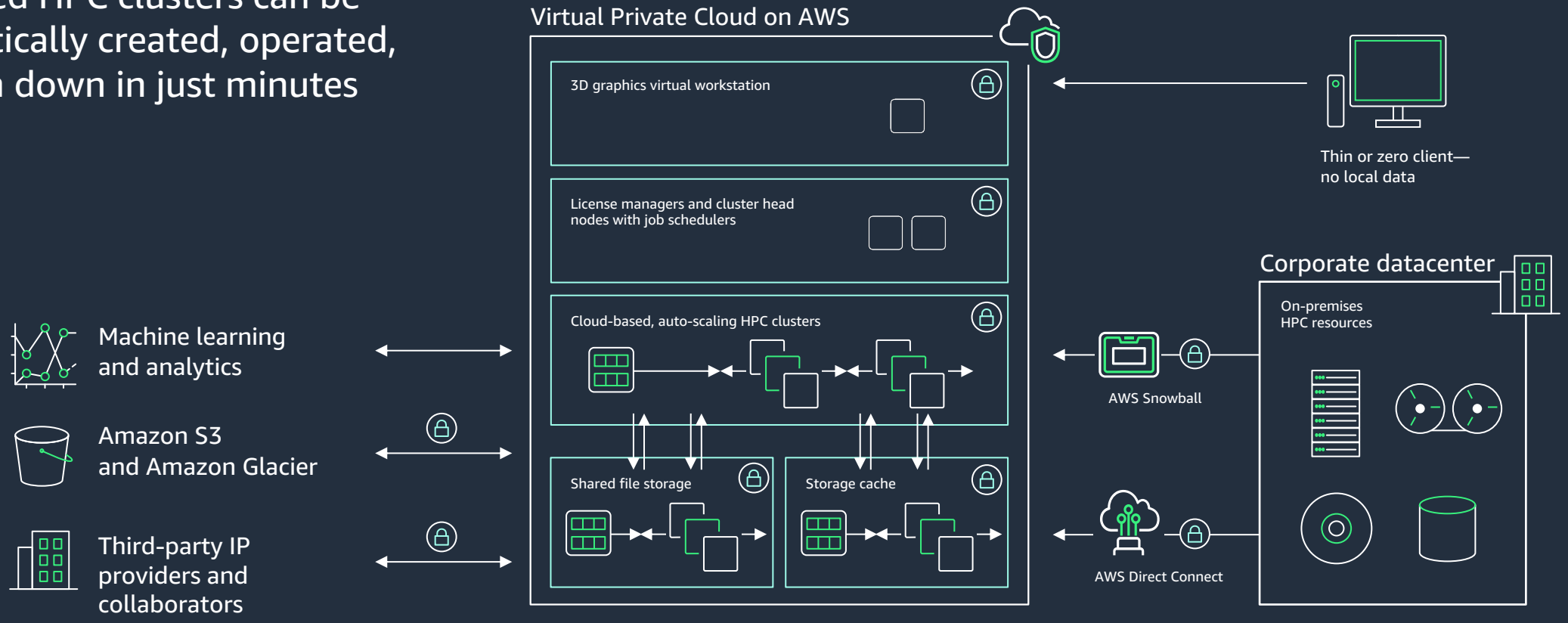
High Performance Computing (HPC) on AWS

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



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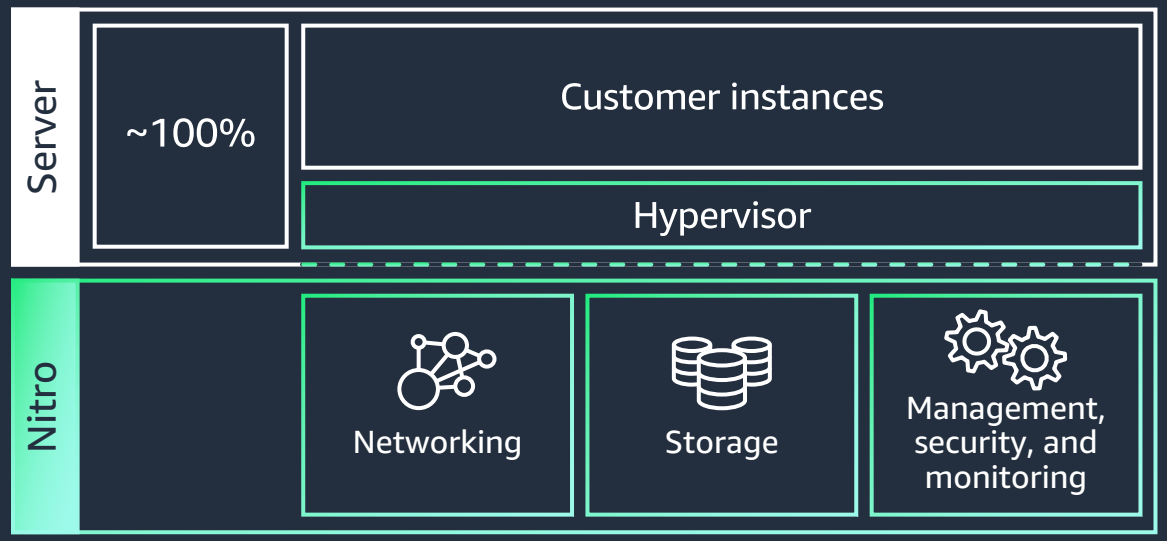
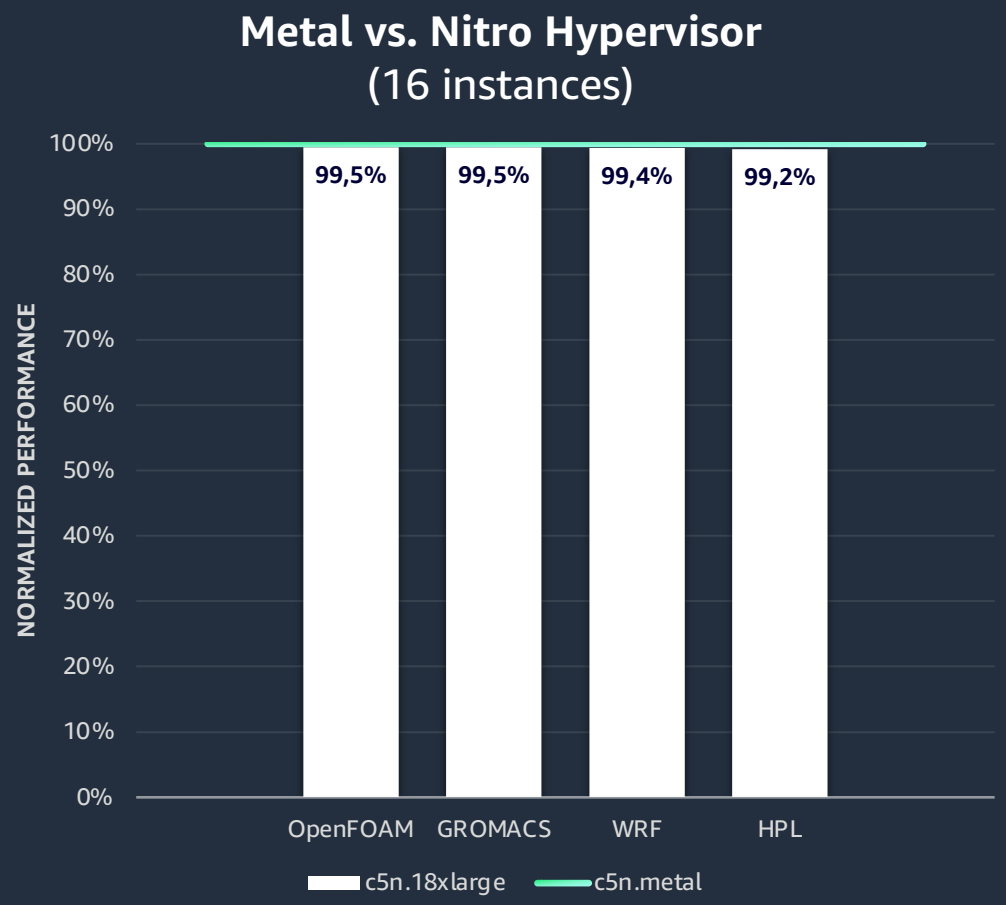
The AWS Nitro System

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





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Amazon EC2 | The compute platform for every workload

Workload types


Machine Learning


High-Performance Computing


Media Rendering


Containers


Web-based Apps


Batch Processing


Big Data

Instance types for HPC workloads

HPC Optimized

Hpc7g | Hpc6a | Hpc6id

Available now

Compute, Memory, and Networking

C7gn | C7g | C6i | M6i

R6i | X2iezn | C5n | M5zn

Accelerators

P4d | G5 | DL1 | Trn1

F1 | Inf1 | VT1

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

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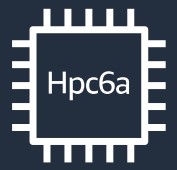
HPC-optimized Amazon EC2 instances

Available now!



Powered by third-generation AMD EPYC processors

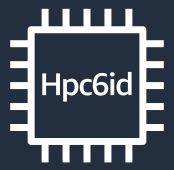
Amazon EC2 Hpc6a instances

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

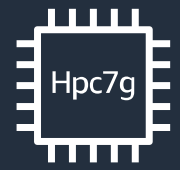
Amazon EC2 Hpc6id instances

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

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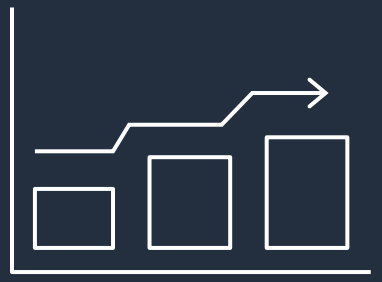
Flexible purchase models to optimize price performance

On-demand

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



Savings Plan

Make a commitment and to save up to 72% off compute for predictable, steady workloads

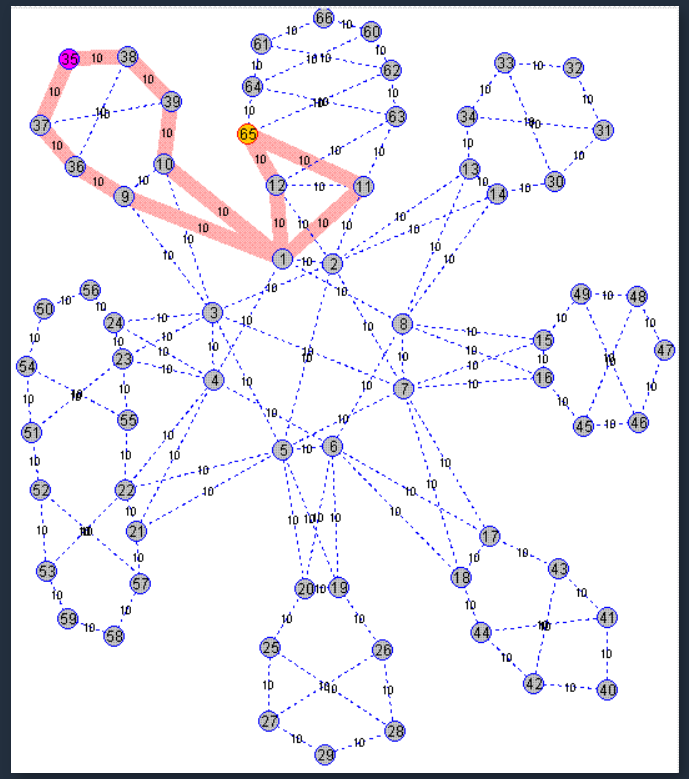
Spot Instances

Spare EC2 capacity at savings of up to 90% off On-Demand prices for stateless, interruptible workloads

Elastic Fabric Adapter—networks built to scale

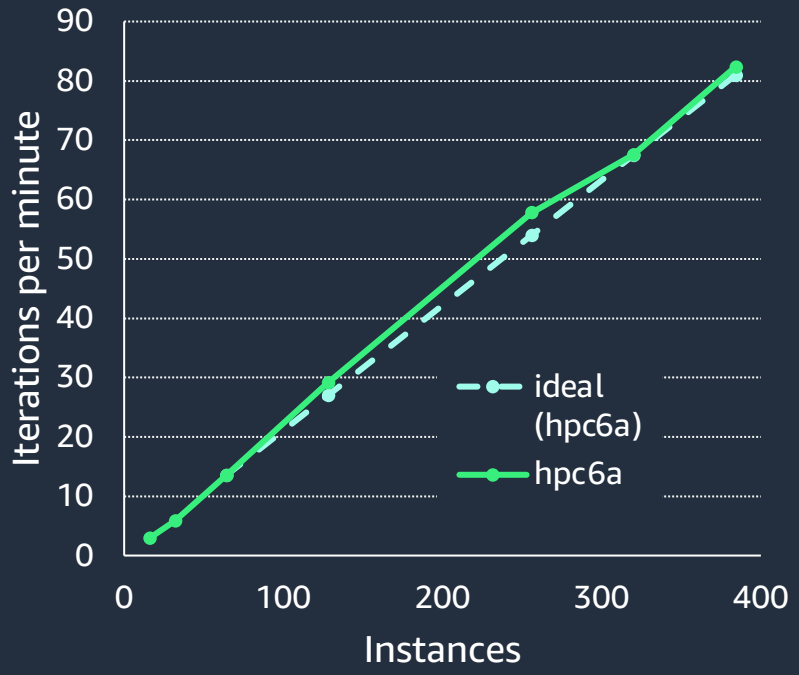
Up to 400 Gbps networking bandwidth

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



ECMP-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

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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

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

Cost-optimized file systems with HDD and SSD storage options

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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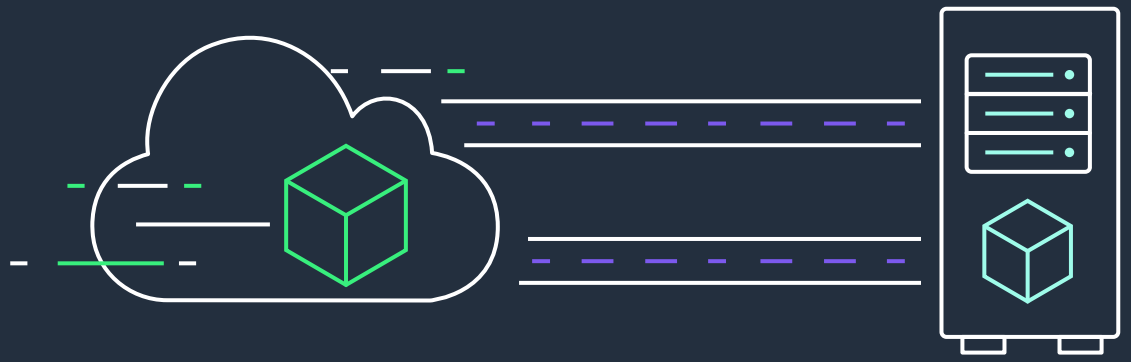
AWS ParallelCluster

One-stop shop to set up your HPC cluster



Integrated with AWS services you need

- Highly-performant file systems
- Amazon EC2 instances
- EFA
- NICE DCV

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NICE DCV

Encrypt and transport pixels to devices

Local clients

Transfer pixels, not data

Remote servers

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

Account and Cluster Setup


Break

AWS Batch and Implementation for Protein Folding

What is AWS Batch?

Job Scheduler

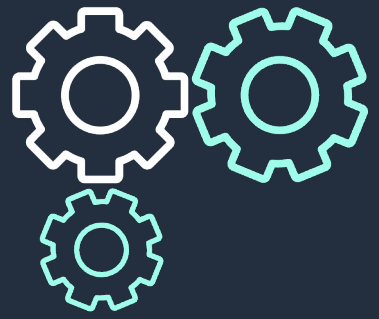
- Schedule & Run jobs asynchronously
- Manages dependencies.

Orchestrator

- Manages & optimizes compute resources
- Scales up/down as needed
- Utilize the right compute resources for the job

Why AWS Batch?

Fully Managed



Integrated with AWS Services

Optimized Resource Provisioning

Cost Efficient

Who uses AWS Batch?

Autonomous vehicle
ML and simulation

Gene sequencing
& Drug Discovery

Big data

Machine Learning

Financial market/
risk analysis

EDA, CAD, FDC

Renewable Energy,
Oil and gas exploration

Weather
simulation

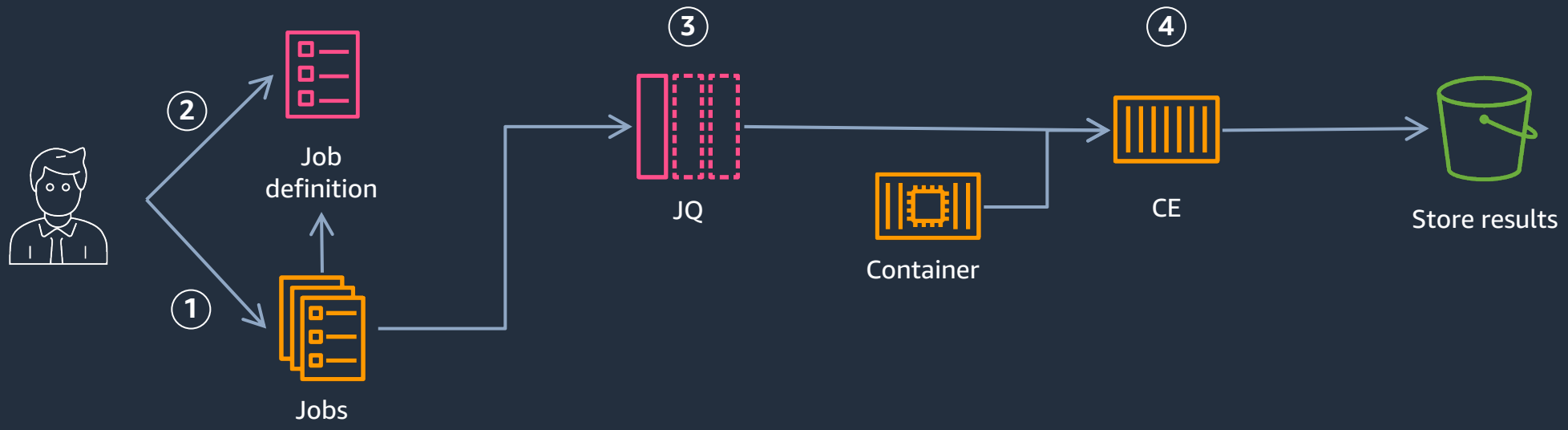
AWS Batch overview

① **Job**
Actual work request – each job must reference a job definition, but many parameters may be overridden when submitted

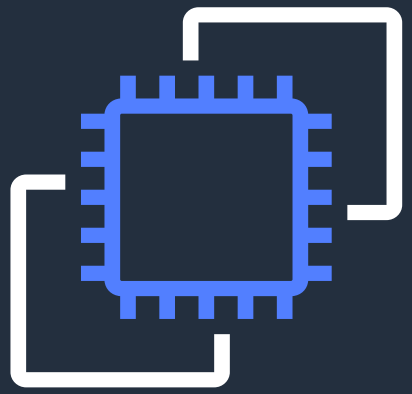
② **Job definition**
Template that has common attributes (such as container image, IAM role, vCPU and memory requirements)

③ **Job queue (JQ)**
Queue determines priorities; each JQ is connected to one or more CE

④ **Compute environment (CE)**
Resource mix (defines On-Demand vs. Spot and other instance types); CE can be connected to more than one JQ

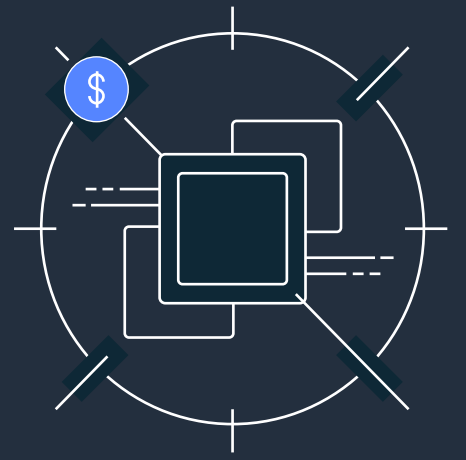


Allocation strategies



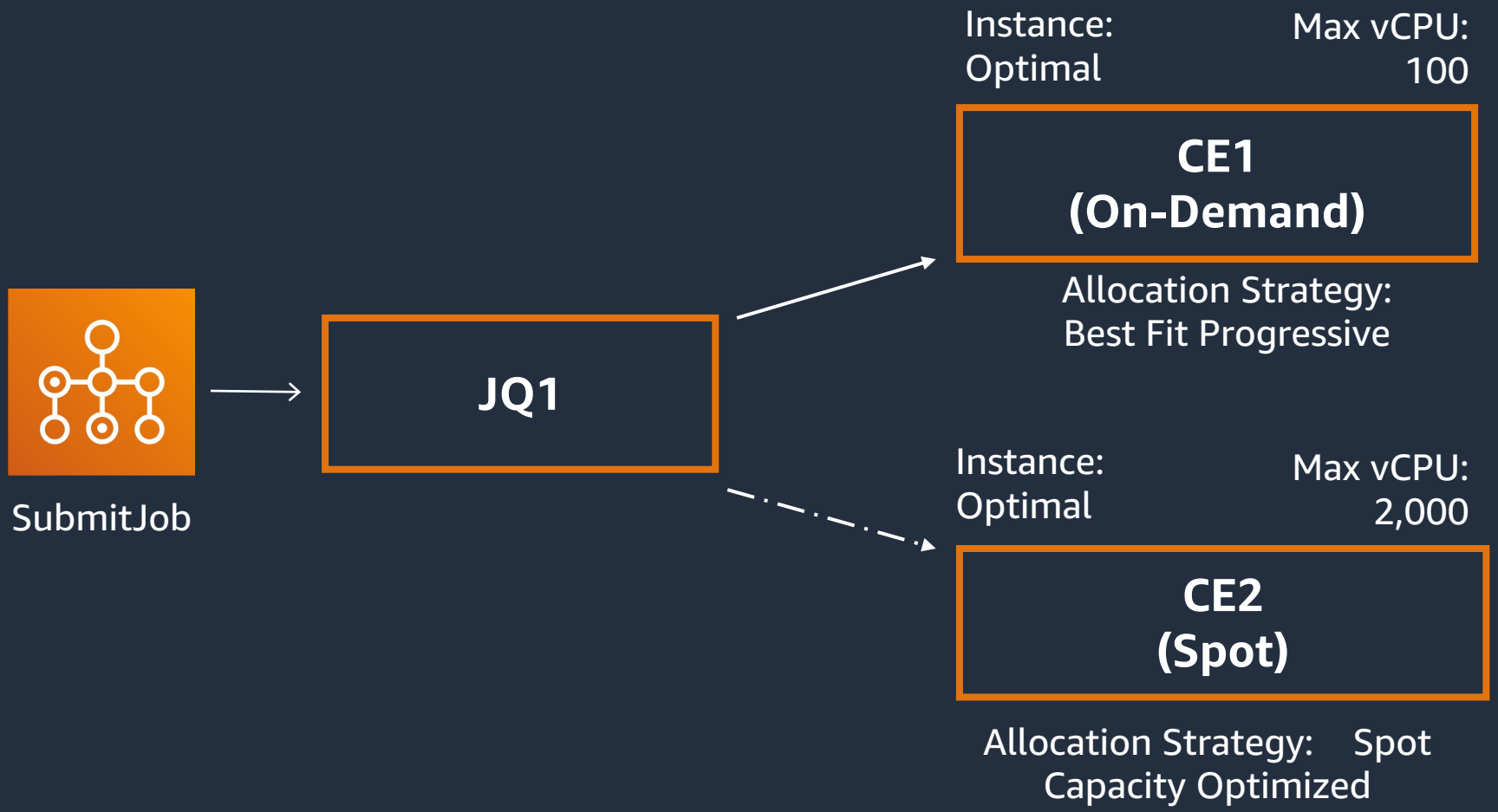
Best Fit

Best Fit Progressive



Spot Capacity Optimized

AWS Batch Allocation strategy example



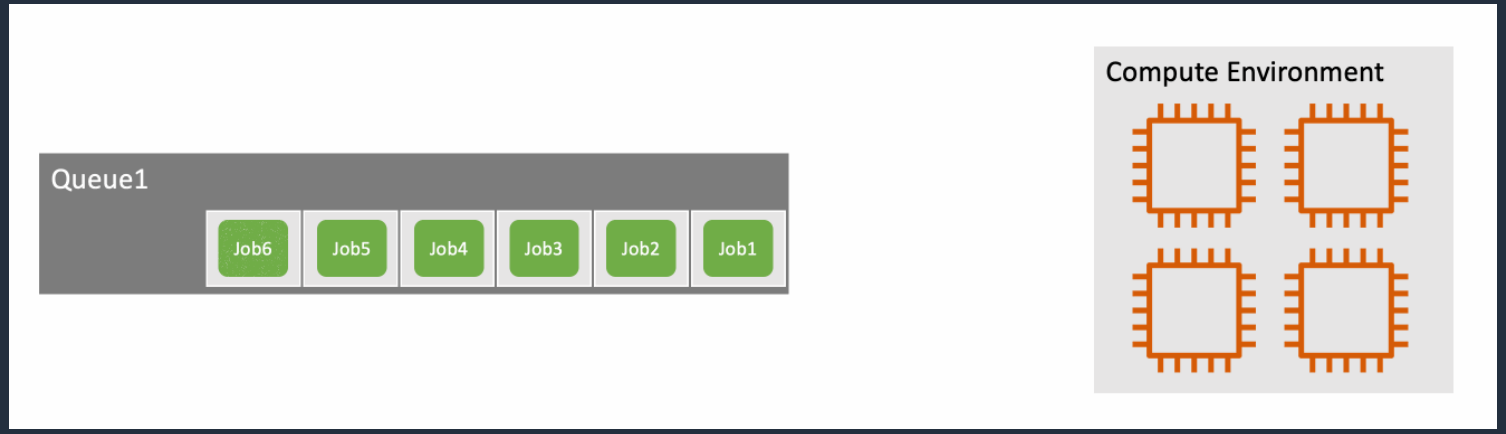
Different execution options

EC2 vs. Fargate?

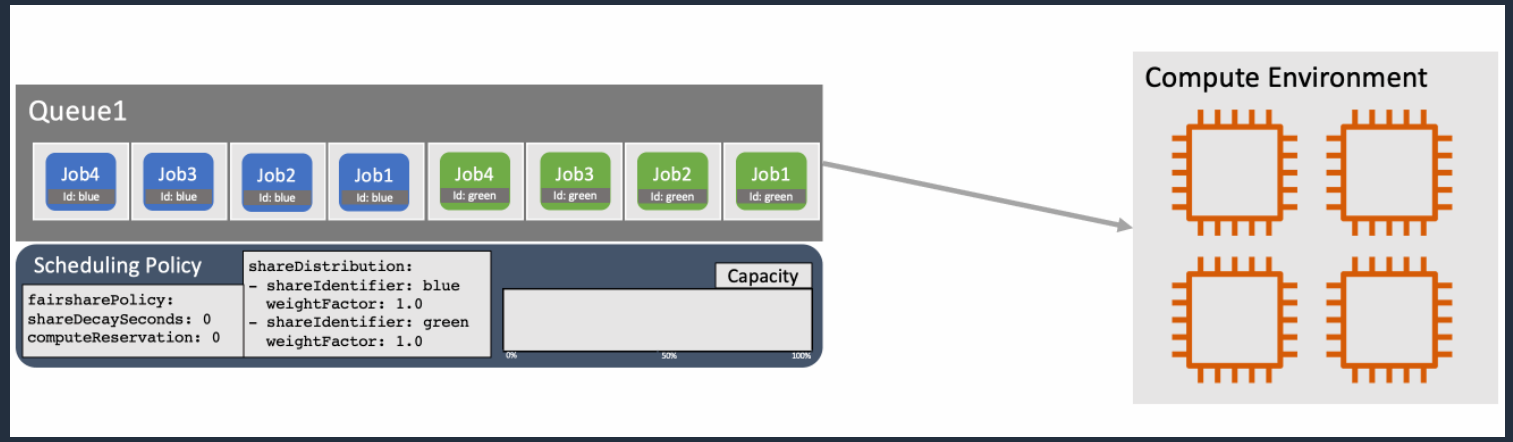
EKS vs. Fargate vs. ECS?

Fair-share scheduling

FIFO

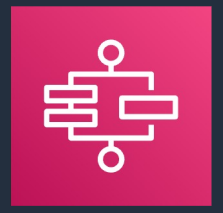


Fair-share



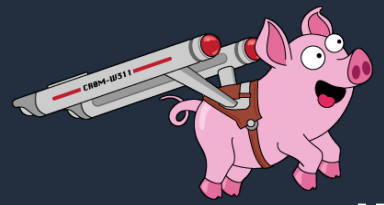
AWS Batch is a natural fit for workflow managers

AWS Native



AWS Step Functions

3rd Party
Open Source



Cromwell

Airflow

Nextflow

Luigi

Sequencing Use Cases

3rd Party
Open Source

Nextflow

Luigi

Flyte

Choosing between AWS Batch or AWS ParallelCluster for your HPC Workloads

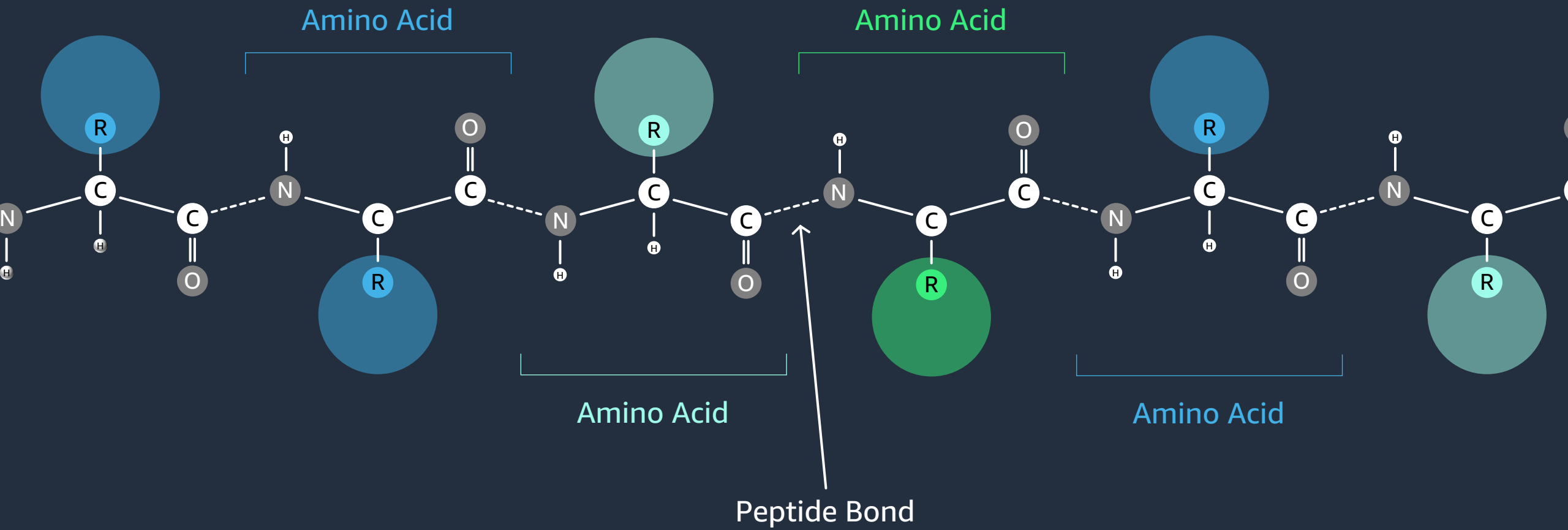
AWS Batch

?

AWS ParallelCluster

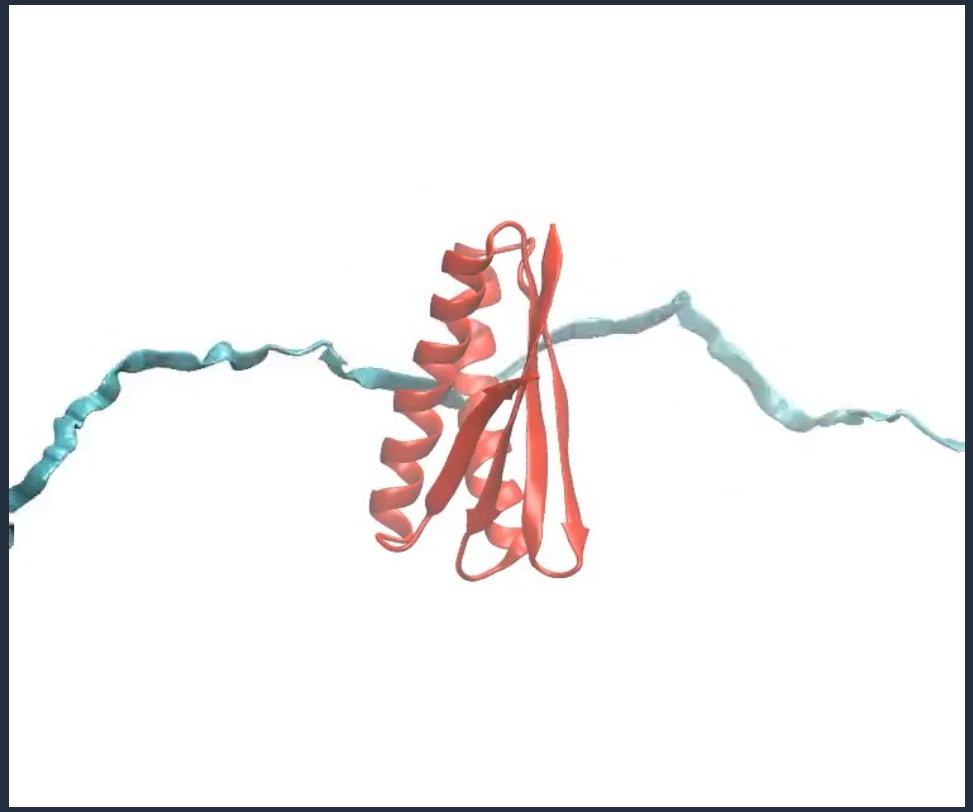
https://s12d.com/GhAuZCLE

What is a protein?



What is protein folding?

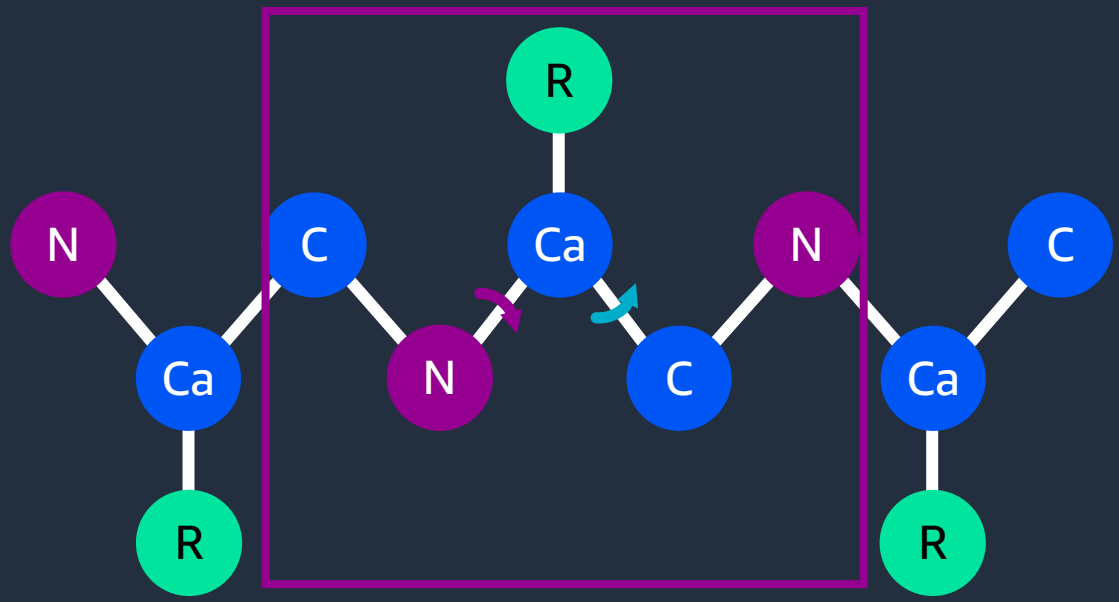
- Protein folding is the physical process by which an unfolded chain folds into a functional 3D protein
- Proteins are synthesized in our body through ribosomes, an RNA-protein complex
- The newly synthesized protein, which is unfolded, must fold into a functional 3D structure



Protein folding video from lab of Dr. Tobin Sosnick, University of Chicago

Levinthal's paradox: Why is protein folding hard?

- 3 major configurations per residue
- For a protein size of 100 residues, there are 3^{100} or 5 x 10^{47} configurations
- At the rate of 10^{13} per second, ~10^{28} years to try all configurations
- Yet, proteins fold in less than a second



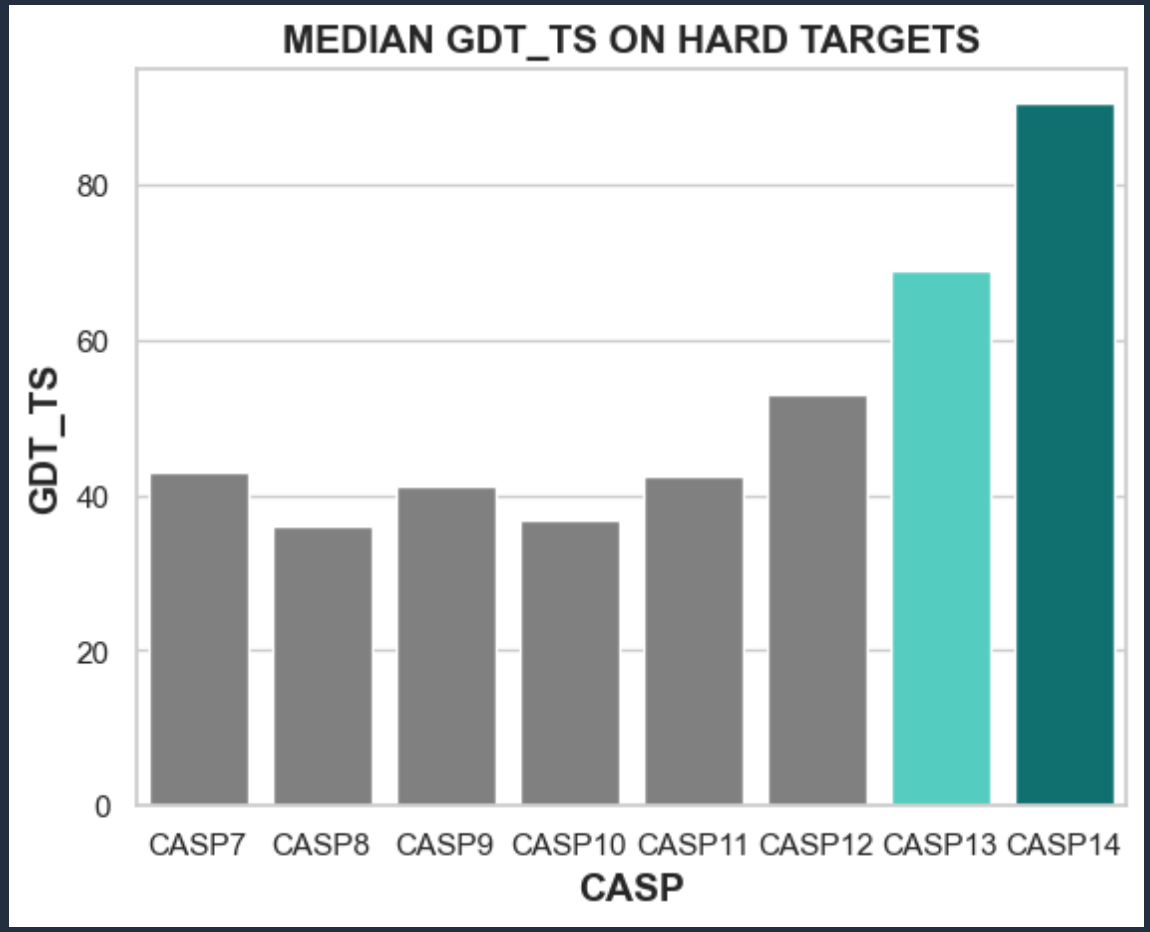
AlphaFold solves protein structure prediction

Article

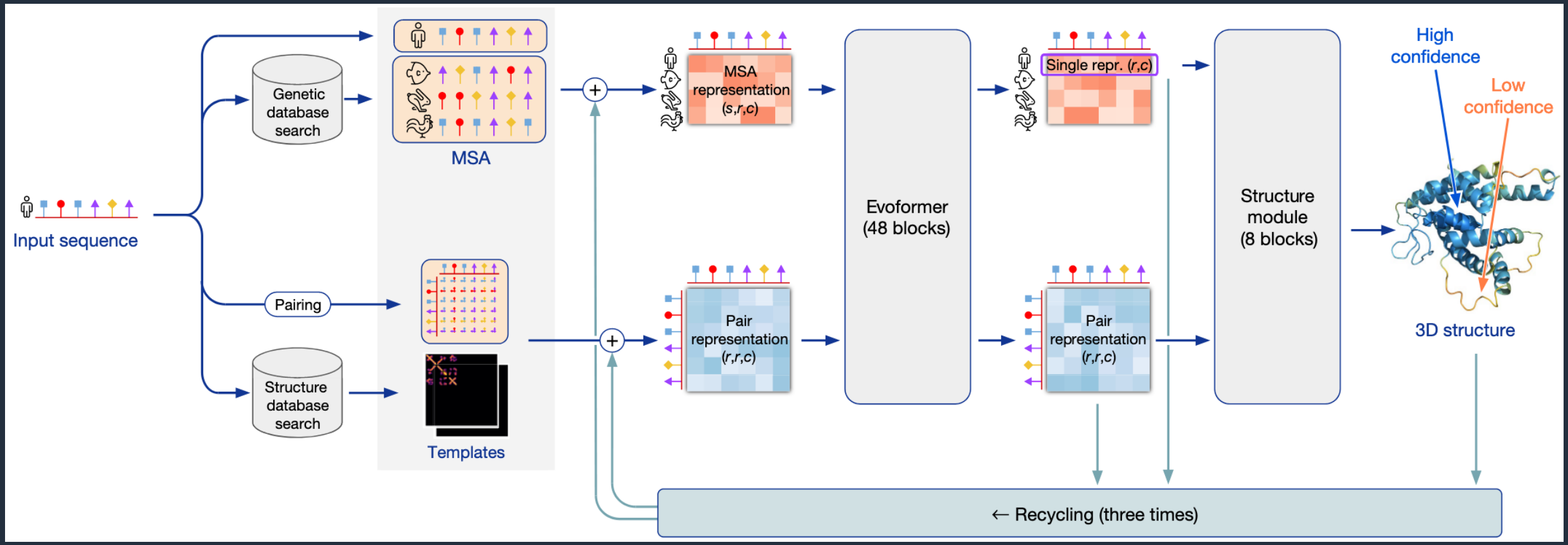
Highly accurate protein structure prediction with AlphaFold

https://doi.org/10.1038/s41586-021-03819-2
Received: 11 May 2021
Accepted: 12 July 2021
Published online: 15 July 2021
Open access
Check for updates

John Jumper[1,4]✉, Richard Evans[1,4], Alexander Pritzel[1,4], Tim Green[1,4], Michael Figurnov[1,4], Olaf Ronneberger[1,4], Kathryn Tunyasuvunakool[1,4], Russ Bates[1,4], Augustin Žídek[1,4], Anna Potapenko[1,4], Alex Bridgland[1,4], Clemens Meyer[1,4], Simon A. A. Kohl[1,4], Andrew J. Ballard[1,4], Andrew Cowie[1,4], Bernardino Romera-Paredes[1,4], Stanislav Nikolov[1,4], Rishub Jain[1,4], Jonas Adler[1], Trevor Back[1], Stig Petersen[1], David Reiman[1], Ellen Clancy[1], Michal Zielinski[1], Martin Steinegger[2,3], Michalina Pacholska[1], Tamas Berghammer[1], Sebastian Bodenstein[1], David Silver[1], Oriol Vinyals[1], Andrew W. Senior[1], Koray Kavukcuoglu[1], Pushmeet Kohli[1] & Demis Hassabis[1,4]✉

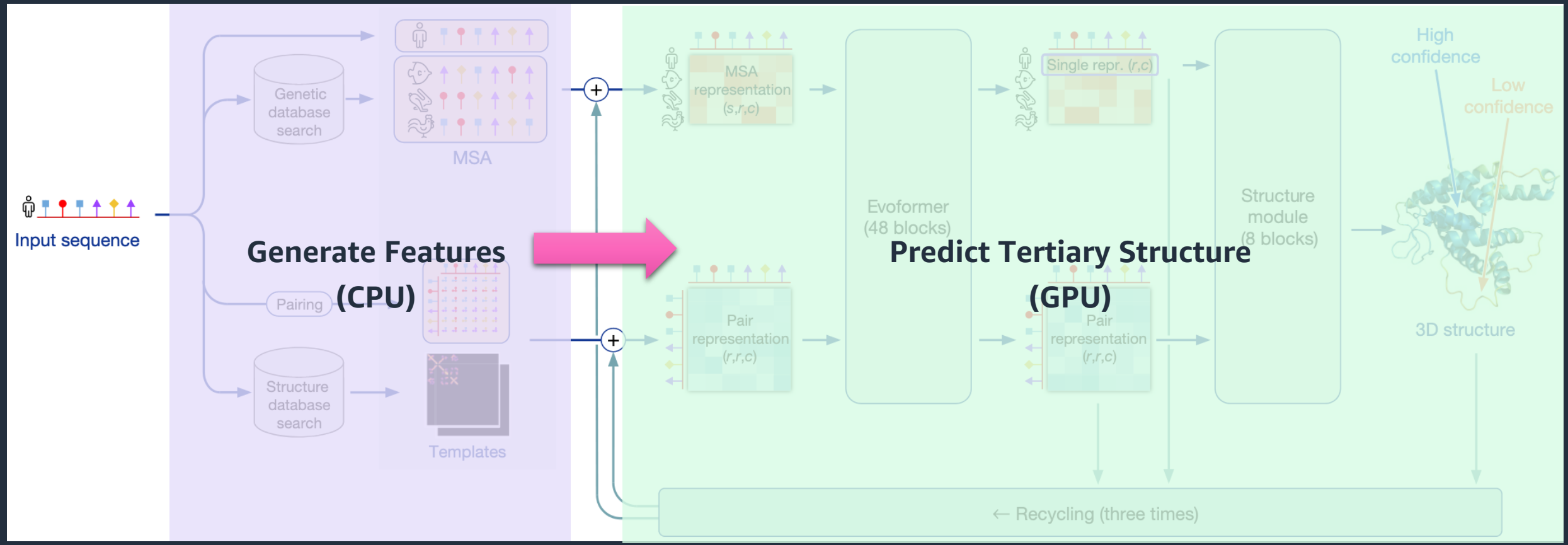


AlphaFold



Jumper, J., Evans, R., Pritzel, A. *et al.* Highly accurate protein structure prediction with AlphaFold. *Nature* 596, 583–589 (2021). https://doi.org/10.1038

AlphaFold Workload Steps Have Unique Requirements



Jumper, J., Evans, R., Pritzel, A. *et al.* Highly accurate protein structure prediction with AlphaFold. *Nature* 596, 583–589 (2021). https://doi.org/10.1038

https://s12d.com/PaGbFmRc

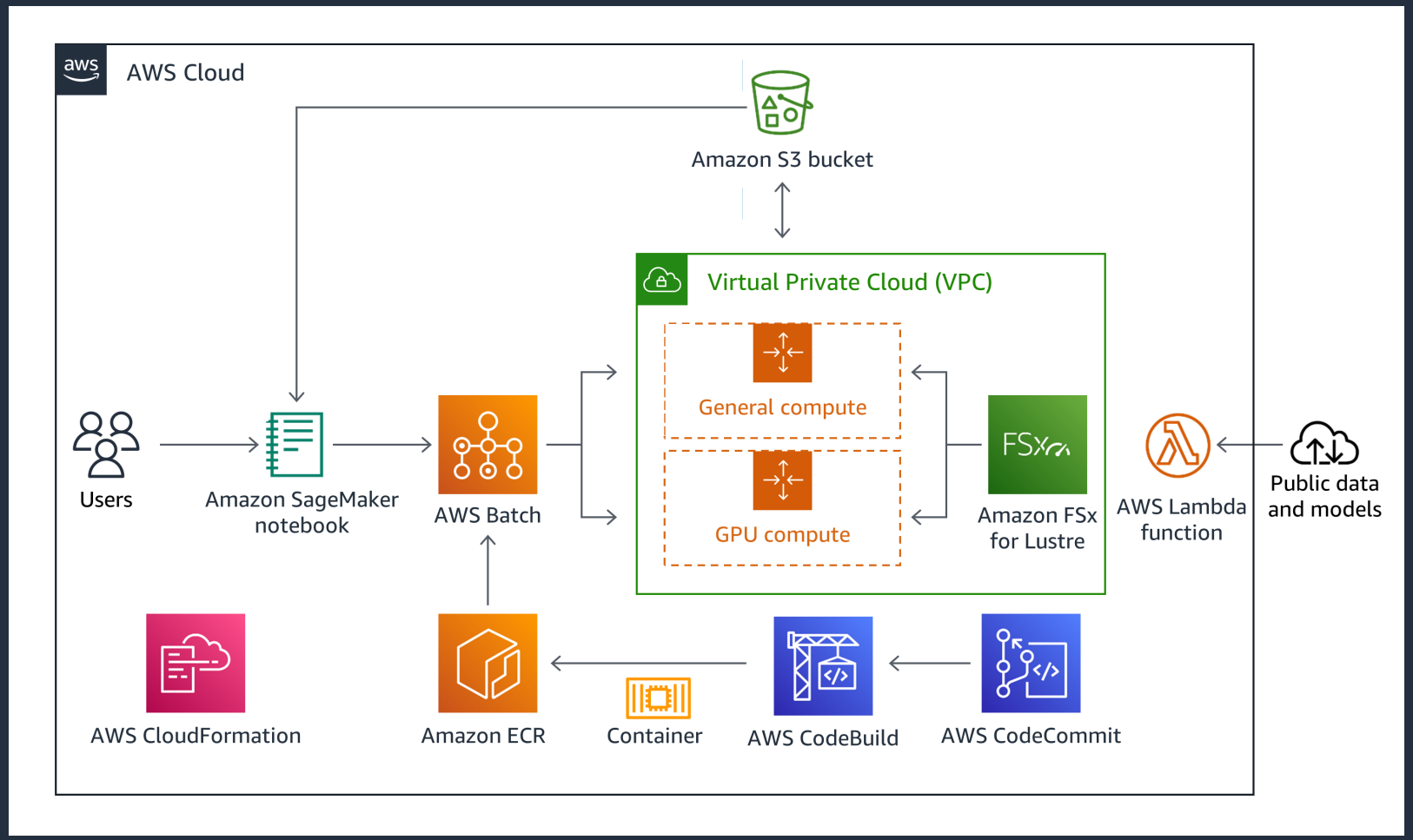
Guidance for protein folding analysis on AWS

NAVIGATE THIS PAGE

This Guidance helps researchers run a diverse catalog of protein folding and design algorithms on AWS Batch. Knowing the physical structure of proteins is an important part of the drug discovery process. Machine learning (ML) algorithms significantly reduce the cost and time needed to generate usable protein structures.

These systems have also inspired development of artificial intelligence (AI)-driven algorithms for de novo protein design and protein-ligand interaction analysis. This Guidance will allow researchers to quickly add support for new protein analysis algorithms while optimizing cost and maintaining performance.

AWS Batch Architecture for Protein Folding and Design



Hands-on Workshop: Molecular Dynamics with GROMACS

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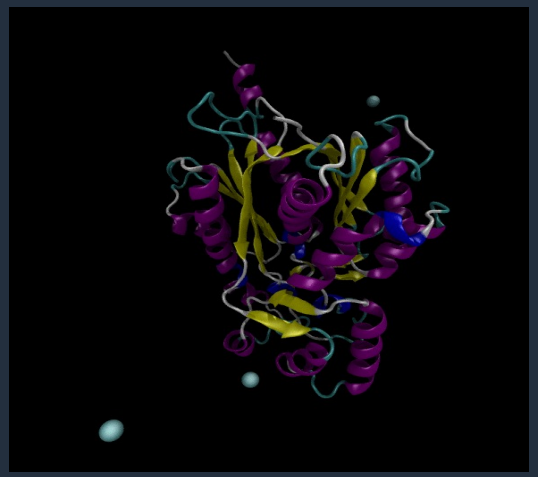
Molecular Dynamics with GROMACS

- Reduce the computation time from weeks to hours
- Optimize across CPU and GPU instances
- Infrastructure as Code: Reproducibility

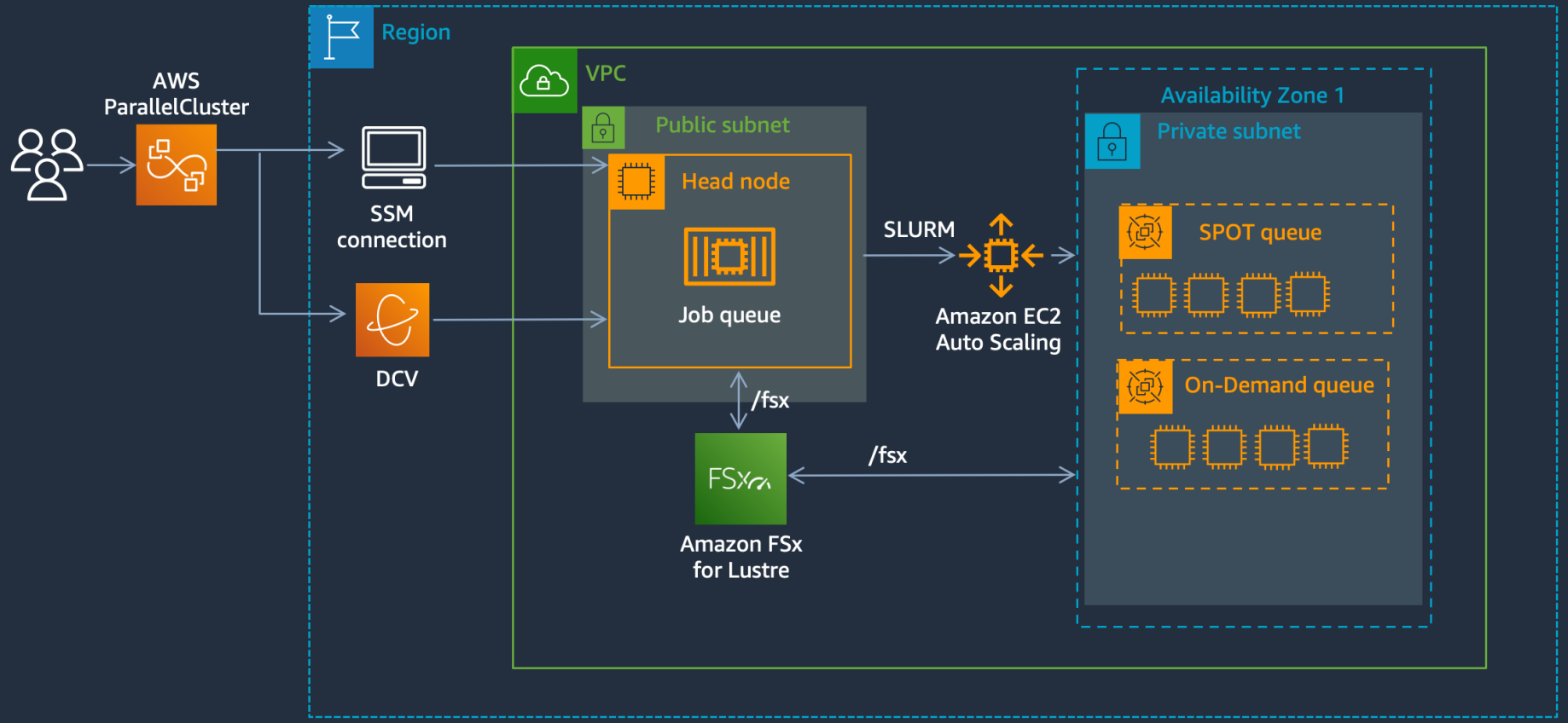
GROMACS Simulation



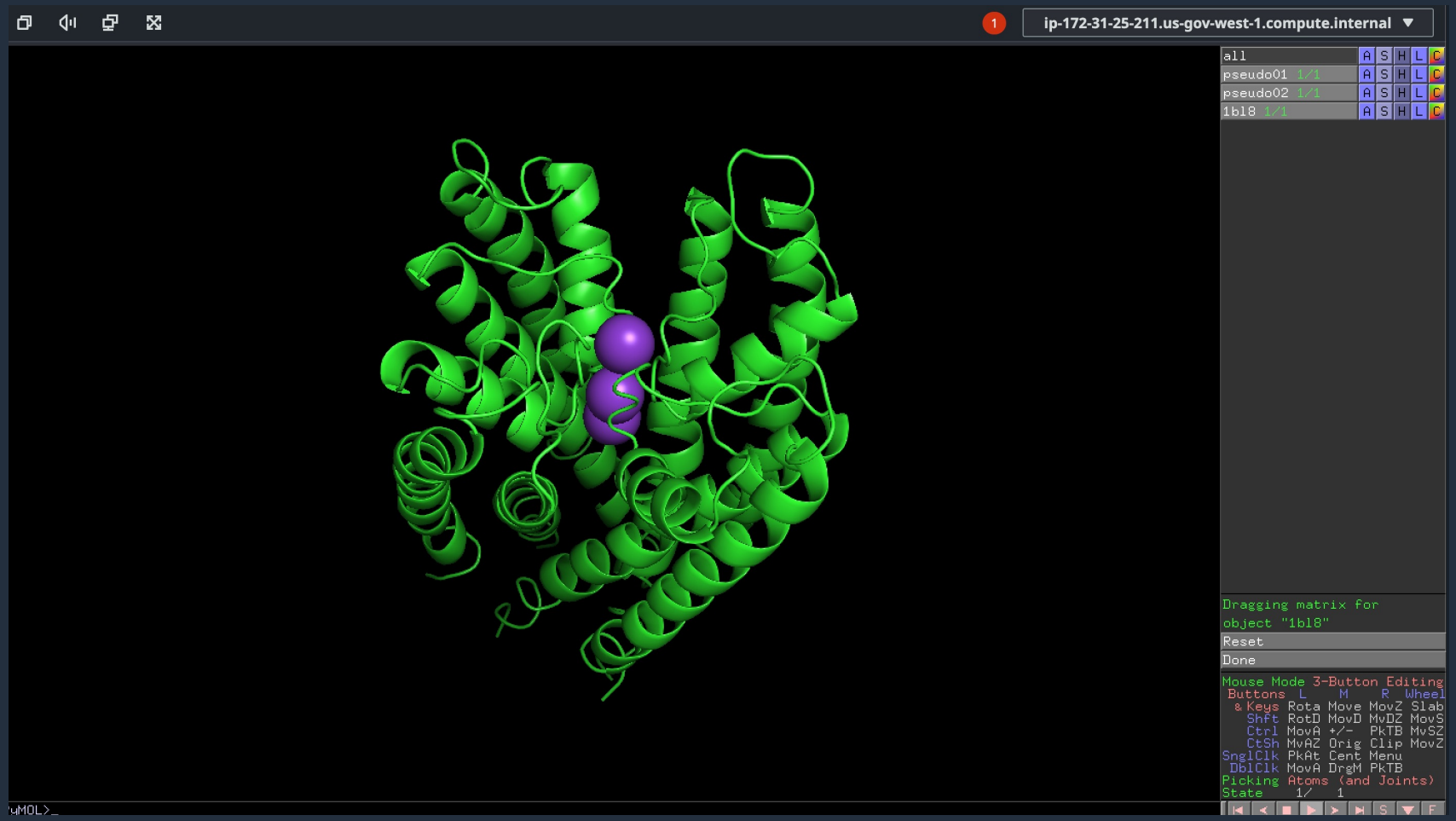
Slurm Workload Manager

- Distributed Resource Management to efficiently manage computing resources in HPC environments.
- Optimization of resource allocation and efficient job scheduling.
- Scalability for large clusters and flexible job prioritization.
- Real-time information on job status and resource usage.

What we will build



Workshop Result



Workshop Instructions

https://s12d.com/wSBuvtHL

Q&A Session

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Please complete the workshop survey

https://s12d.com/6UMF89g1

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https://aws-experience.com/

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- July 6th: Security, Encryption & Data Protection Immersion Day
- July 11th: Sustainability
- **July 13th: High-performance computing**
- July 18th: Compliance in the Cloud

aws health

Thank you!

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Appendix

HPC workloads across industries

Life Sciences

Financial Services

Energy

Automotive

Climate & Earth Sciences

Design & Engineering

Numerix scales HPC workloads for price and risk modeling using AWS Batch

Challenges

Numerix needed to scale its high performance computing (HPC) solution because financial portfolios became overly complex, and as a result, the computing requirements of risk calculations were impeding sales

Solutions

Numerix increased the performance of its financial risk analytics significantly using AWS solutions—migrating to AWS has made it simple for Numerix to scale along with capital markets

Results

- 180x improvement in analytics performance
- Enhanced risk management
- Decreased bottlenecks in analytics

> "Our clients are using our risk analytics to avoid billion-dollar losses. The introduction of near-real-time analytics with the virtually limitless scalability of AWS has been a real game changer."
>
> **Jim Jockle**
> Chief Marketing Officer, Numerix

CUSTOMER PROFILE

numerix

INDUSTRY
Financial Services

REGION
United States

Founded in 1996, Numerix is a financial technology company headquartered in New York City, with 16 offices in 16 countries—it provides analytics software for more than 250 global clients, including banks, regulators, and insurance companies

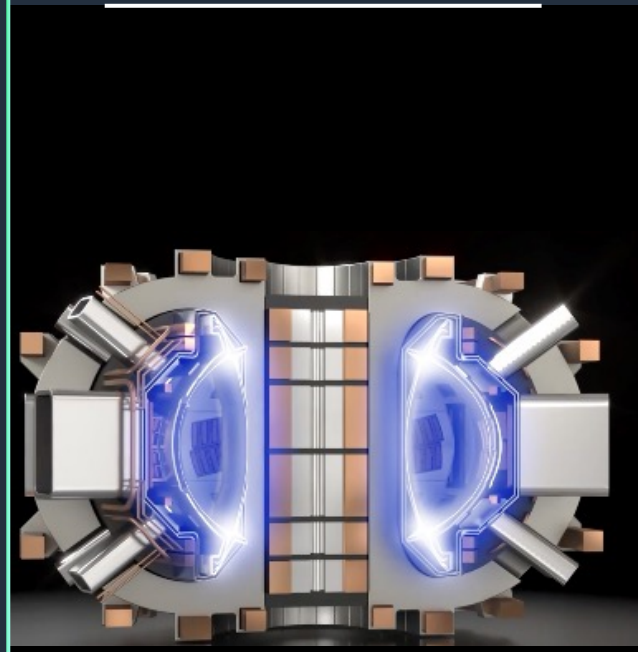
aws

Commonwealth Fusion Systems (CFS)

CUSTOMER PROFILE

Commonwealth Fusion Systems

- 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

aws

Formula 1 redesigns car for closer racing and more exciting fan experience

CUSTOMER PROFILE

Formula1 runs its Computational Fluid Dynamics (CFD) platform on AWS HPC

- Reduces downforce loss in wheel-to-wheel racing from 50 percent to 15 percent reducing the impact of the car in front of it
- Better supports strategic priorities for increasing competitiveness and unpredictability on the track
- Cars can drive closer to one another and overtake more easily creating a world-class spectacle for fans

Lowered the cost of CFD simulations by 30%

Reduced CFD simulation time by 80%

aws

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

DTN

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

aws

Creating air taxi simulations using Amazon EC2 with Wisk Aero

Challenges

Wisk Aero relies on high performance compute (HPC) to run computationally intensive and complex simulations, each of which uses thousands of CPU cores. Purchasing on-premises computers for its HPC workload presented several challenges

Solutions

Wisk Aero has developed the first-ever autonomous electrical vertical take-off and landing (eVTOL) aircraft and is using Amazon Web Services (AWS) to build HPC clusters to run simulations

Results

- 10–20% improvement in job runtime
- Satisfies NASA software requirements
- Achieves high-performance, scalable storage
- Drives improved economics

> "Using AWS, we quickly scaled and added the needed on-demand compute power for the CFD team, compared with the months required and significant capital to build and scale an on-premises HPC cluster."

Colin Haubrich
Head of IT, Wisk Aero

CUSTOMER PROFILE

wisk

INDUSTRY
Aerospace

REGION
United States

Wisk Aero is an advanced air mobility company dedicated to delivering safe, everyday flight for everyone—the company is backed by the Boeing Company and Kitty Hawk Corporation

aws

Broad HPC partner community

Software Partners

AMD
ALTAIR
Ansys
arm
CFD Direct
cadence
DASSAULT SYSTEMES
HEXAGON
IBM
illumina
intel
NVIDIA
Parallel Works
rescale
RONIN
S-CUBE
SIEMENS
SIMSCALE
slurm | SchedMD
SYNOPSYS
TECHILA
TotalCAE
YELLOWDOG
ZENOTECH SIMULATION UNLIMITED

Consulting Partners

Atos
CADFEM
Clovertex modernization made simple
Cognizant
DXC.technology
OCF
six nines
X-ISS

aws

AWS Best HPC Cloud Platform for 5 years running

AWS Batch

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

Compliance programs

Global

SOC 1


SOC 2


SOC 3


Europe


Asia Pacific

United States





aws

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