

The background features a dark blue gradient with abstract geometric shapes. On the left, a large triangle is formed by a vertical orange line and a diagonal orange line. On the right, a large curved shape in shades of blue and orange sweeps across the frame. The text is positioned in the upper right area.

AWS re:Invent

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

CMP312

The future of HPC is looking a lot like ML

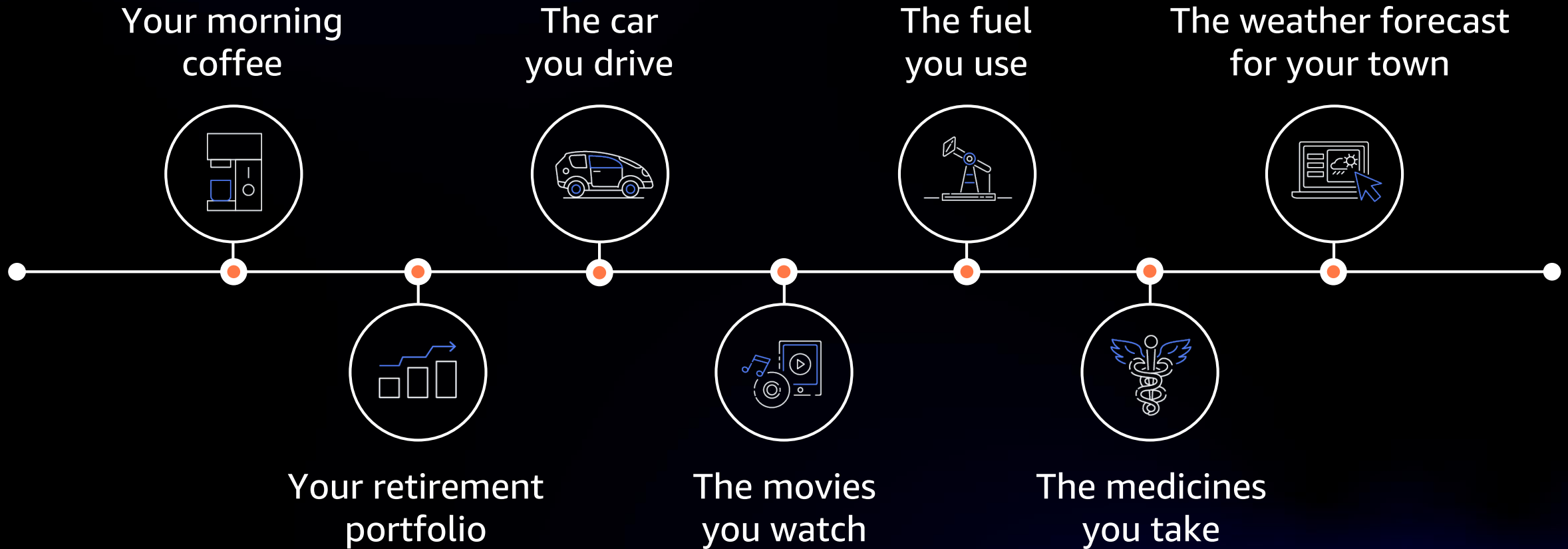
Barry Bolding (he/him)
Director HPC, Quantum, and
Autonomous Computing
AWS

Jyothi Venkatesh (she/her)
HPC Specialist Solutions Architect
AWS

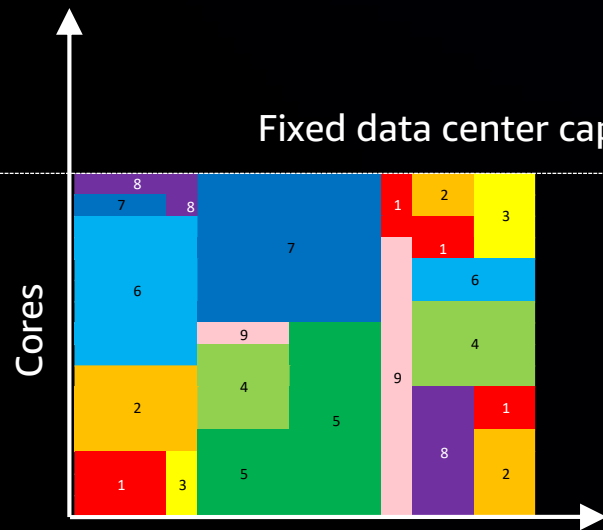
Terry Cunningham (he/him)
CEO
Descartes Labs



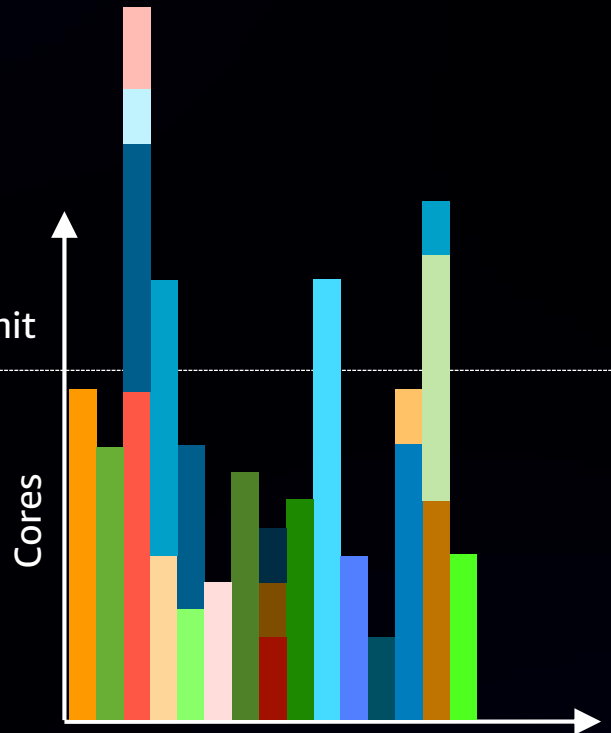
High performance computing (HPC) impacts your life every day



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



Finite capacity, usually with long queues to wait in



Massive capacity when needed to speed up time to results, and agile environment when additional hardware and software experimentation is needed

"For every \$1 spent on HPC, businesses see \$507 in incremental revenues and \$47 in incremental profit."*

Working backward: The Amazonian way

Working backward from customer requirements

Functional asks



Faster development cycles



Tools to derive insights



Easier access to data

Operational asks

Security, data governance



Cost management



Data transfer and management

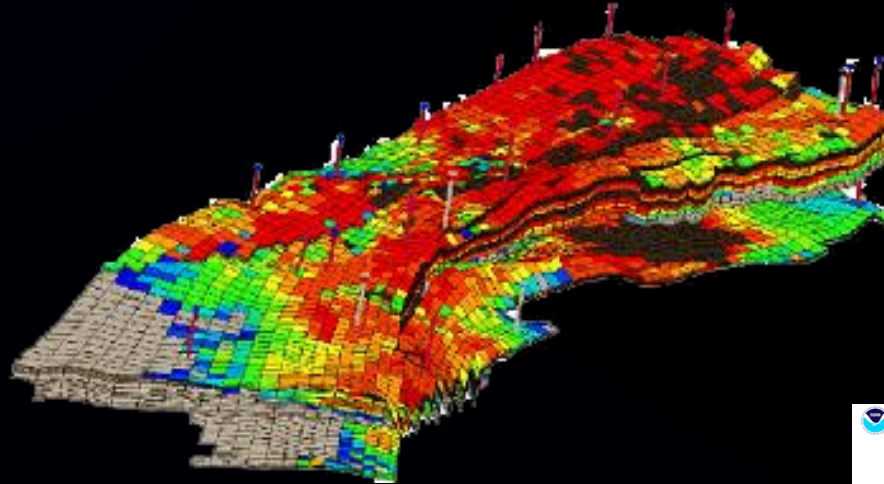


aws

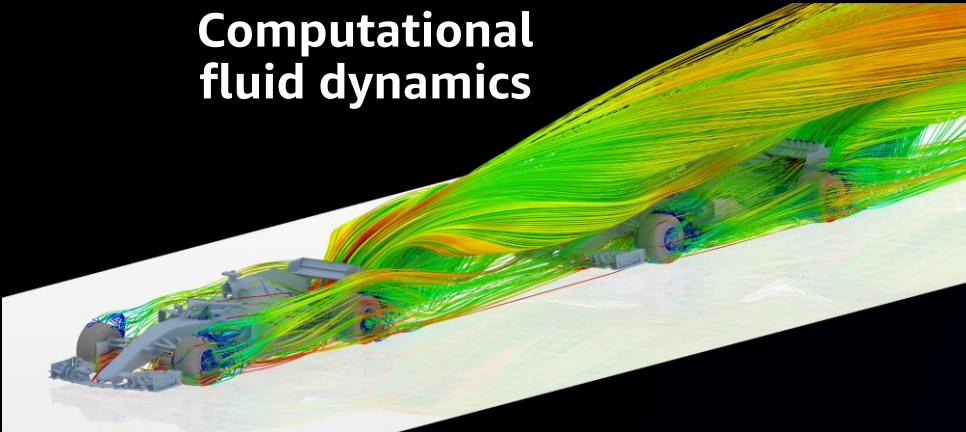
New: Can I derive increased business value from machine learning (ML) + HPC?

Any type of HPC workload is possible on AWS

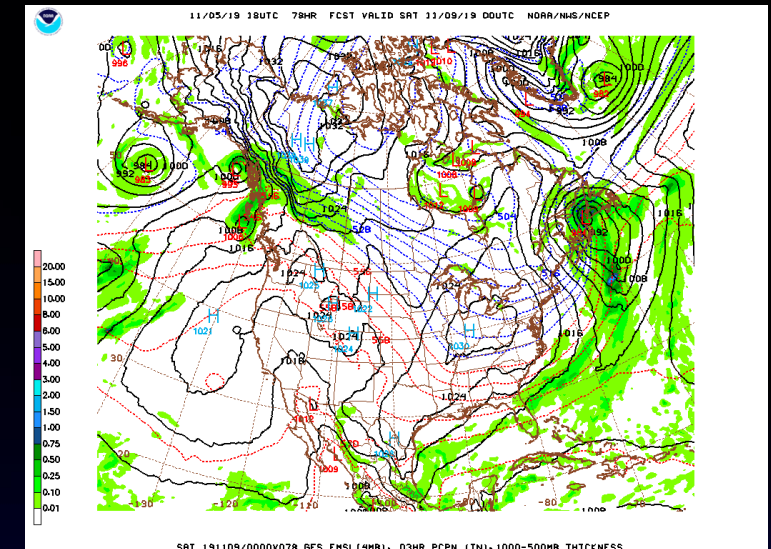
Reservoir simulations



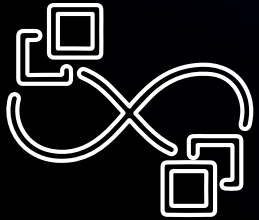
Computational
fluid dynamics



Weather forecasting

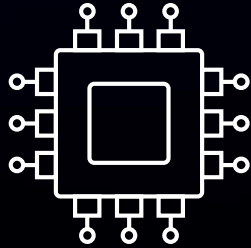


Key services that enable HPC on AWS



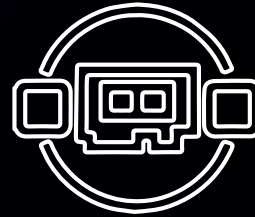
Visualization

AWS
ParallelCluster



Compute

Amazon EC2



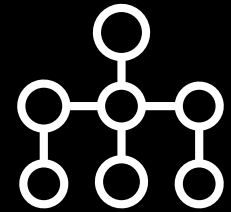
Networking

Elastic Fabric
Adapter (EFA)
+
up to 400 Gbps
networking



Storage

Amazon FSx
for Lustre and
Amazon FSx for
NetApp ONTAP



Orchestration

AWS Batch

AWS
ParallelCluster

EnginFrame

AWS takes a systemic view of workload

Broadest choice of processors in the cloud

The Intel logo, featuring the word "intel" in a lowercase, sans-serif font with a small blue square above the "i".

Intel Xeon Scalable
(Skylake and Cascade
Lake) processors

The AMD logo, featuring the word "AMD" in a bold, sans-serif font followed by a stylized square icon.

AMD EPYC (Naples and
Rome) processors

The AWS logo, featuring the word "aws" in a lowercase, sans-serif font with a curved orange arrow underneath.

AWS Graviton2
processor

Modular building blocks for rapid design and delivery of EC2 instances

Broadest choice of accelerators in the cloud



NVIDIA V100 Tensor
Core and T4 Tensor
Core GPUs



Xilinx FPGAs for
custom hardware
acceleration

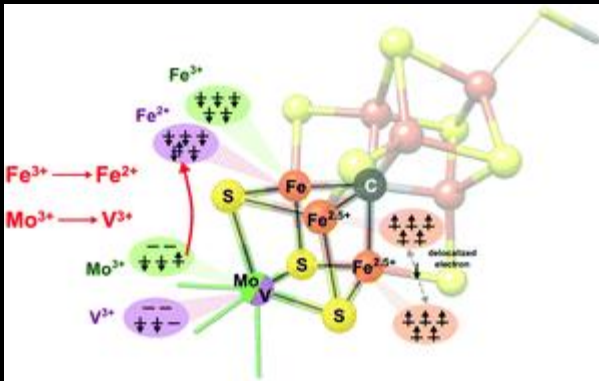


AWS Inferentia for
ML inference

Right accelerator for any workload

The disruptive potential of quantum computing

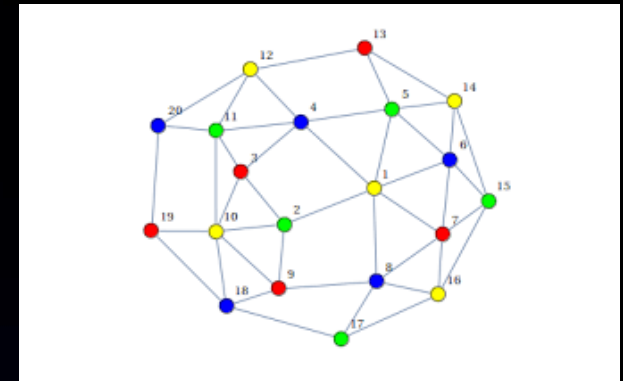
Quantum computing holds the promise to speed up solutions to hard problems



Computational chemistry



Machine learning

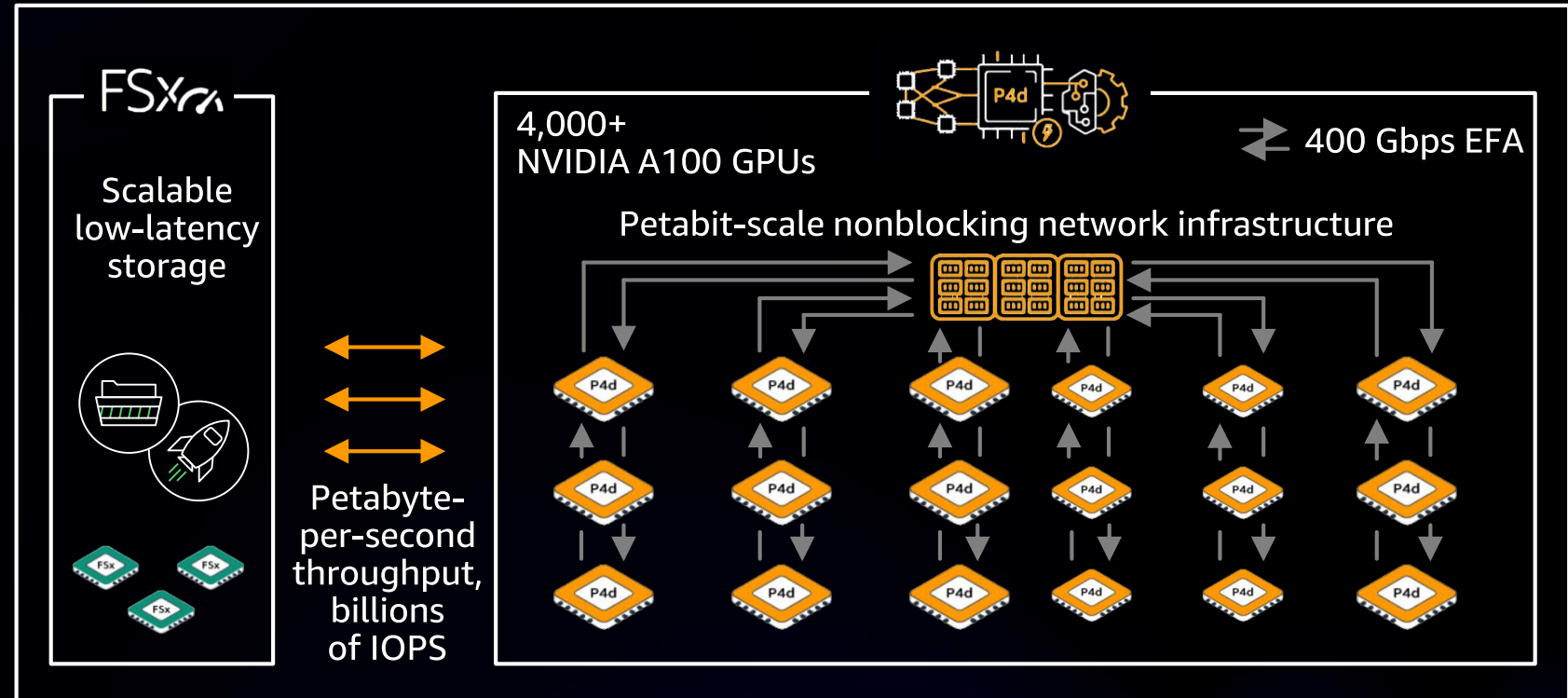


Optimization

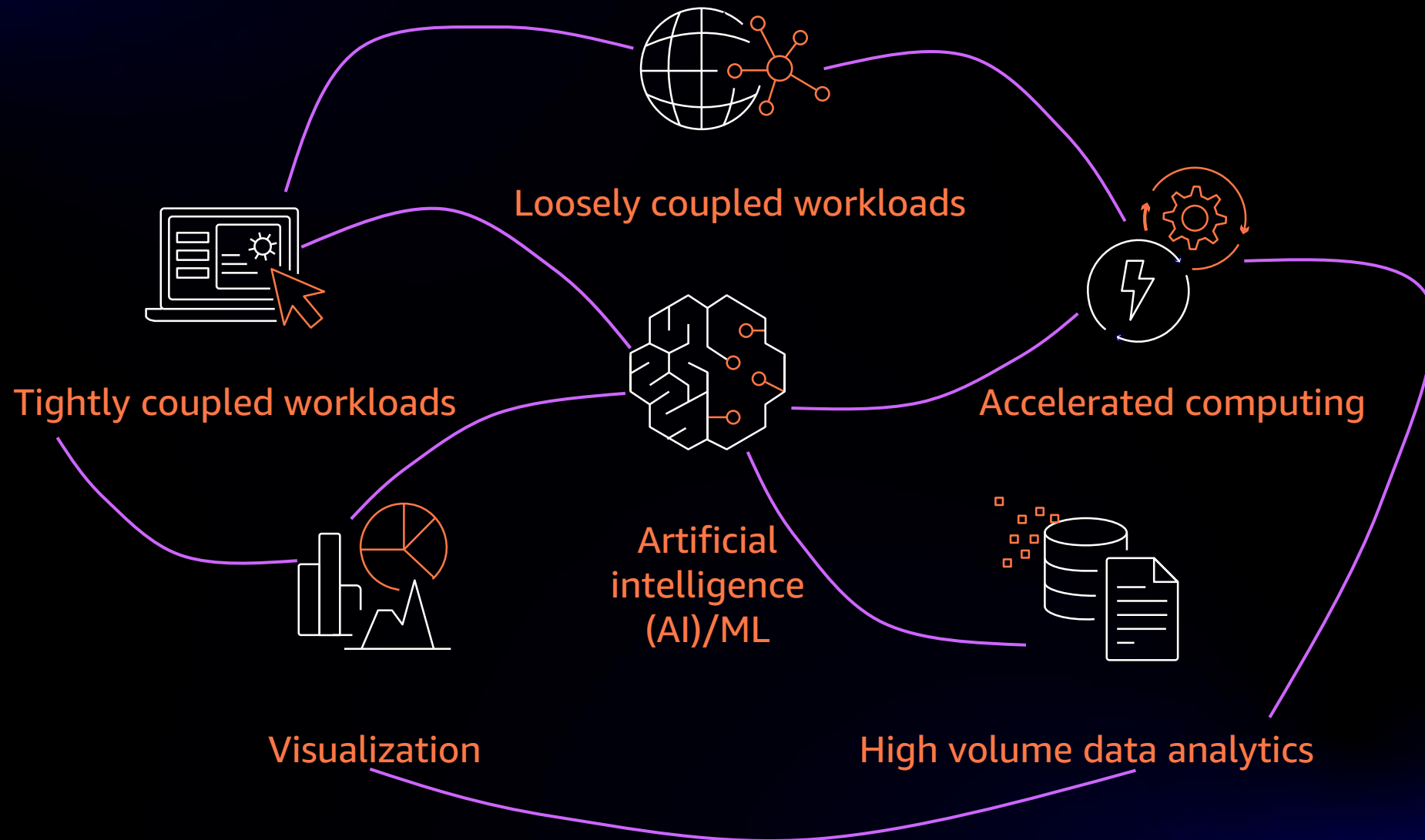
EC2 UltraClusters: Supercomputing-class performance for HPC and ML/DL

- Based on NVIDIA A100 graphics processing units (GPUs)
- Availability to scale out to large clusters for distributed training
- 2.5x better deep learning (DL) performance and 60% lower cost to train
- EC2 UltraClusters with EFA enable 400 Gbps and allow you to scale to over 4,000 GPUs

EC2 UltraClusters

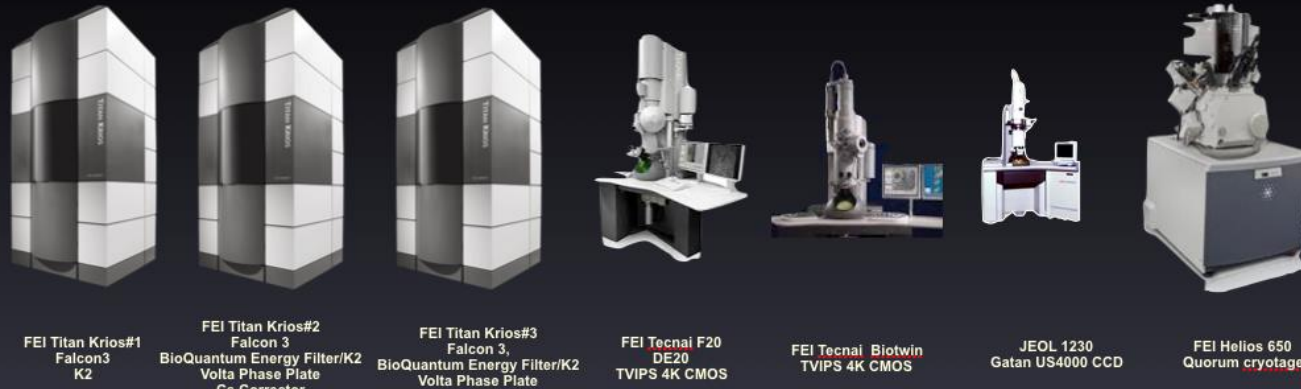


Varied compute and throughput characteristics

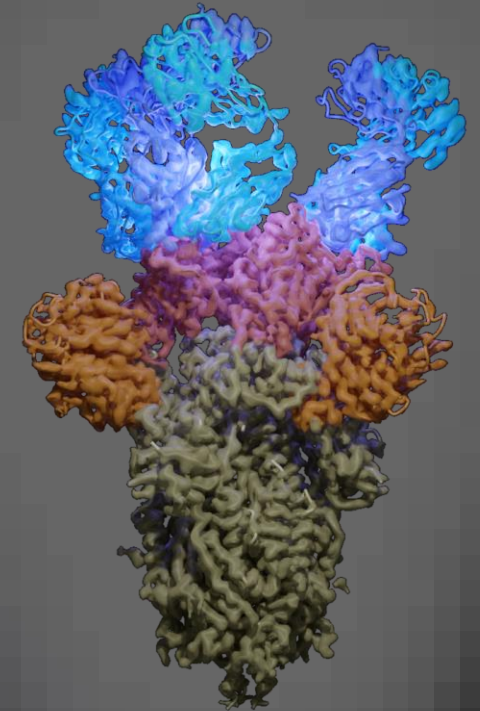
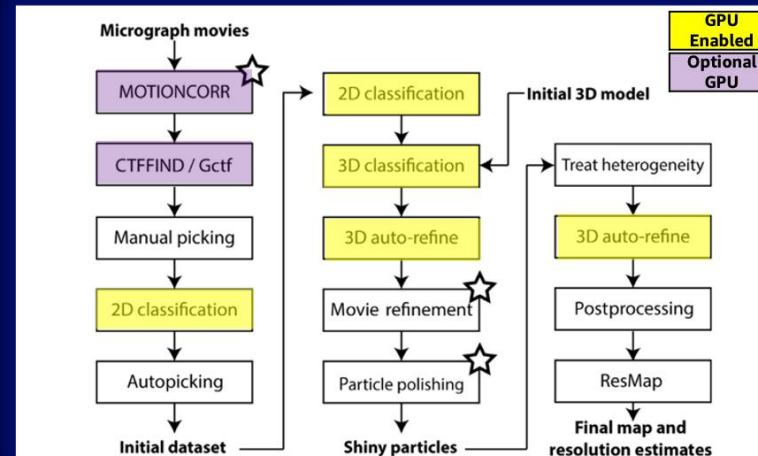
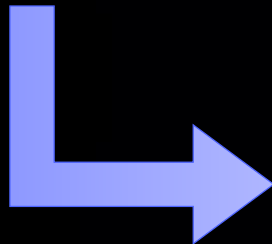


Cryo-Electron Microscopy (Cryo-EM)

SEMC Major Instrumentation



<https://nramm.nysbc.org/infrastructure/>



Antibody 2-4
Liu et al., *Nature* 2020
PDB 6XEY

[10.1038/s41586-020-2571-7](https://doi.org/10.1038/s41586-020-2571-7)
Structure courtesy of Micah Rapp

Case study: Boom Supersonic

GOES ALL-IN ON AWS



Boom Supersonic used AWS to **accelerate the design and construction** of its supersonic aircraft

Boom can run thousands of advanced computer simulations concurrently, resulting in an estimated **6x increase in productivity versus an on-premises environment**

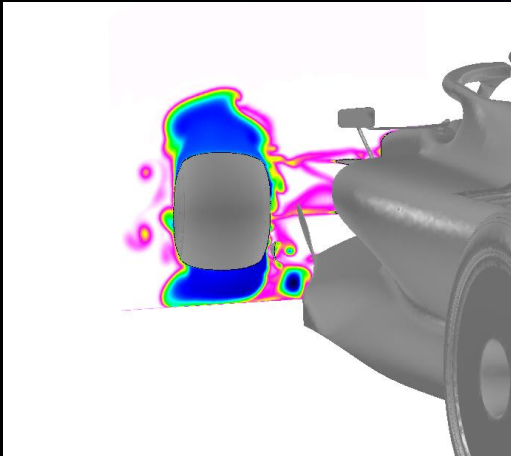
Boom used more than **53 million compute hours** on AWS to **complete design and testing** of its Overture airliner

"AWS, the world's leading cloud provider, will help us continuously refine our designs."

Blake Scholl, Founder and CEO, Boom Supersonic

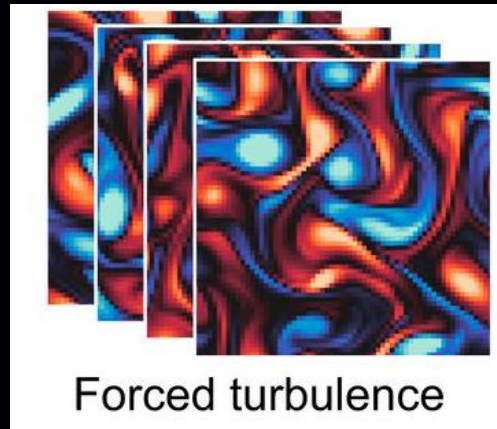
ML + HPC possibilities

Extract relationships
from simulation data



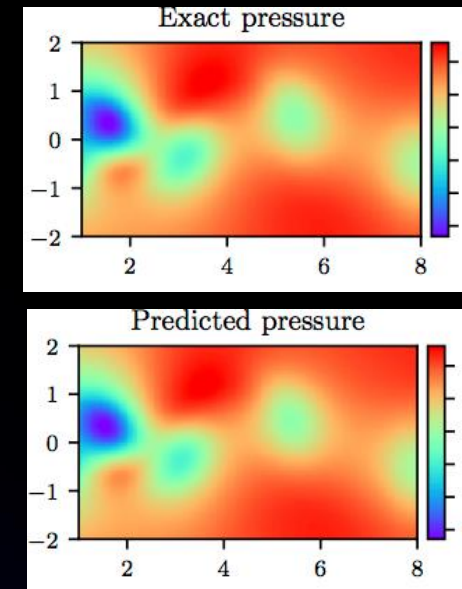
Credit: F1

Accelerate HPC simulations
with embedded ML models



Credit: "Machine learning–accelerated computational fluid dynamics,"
<https://www.pnas.org/content/118/21/e2101784118>

Learn solutions to governing
equations directly

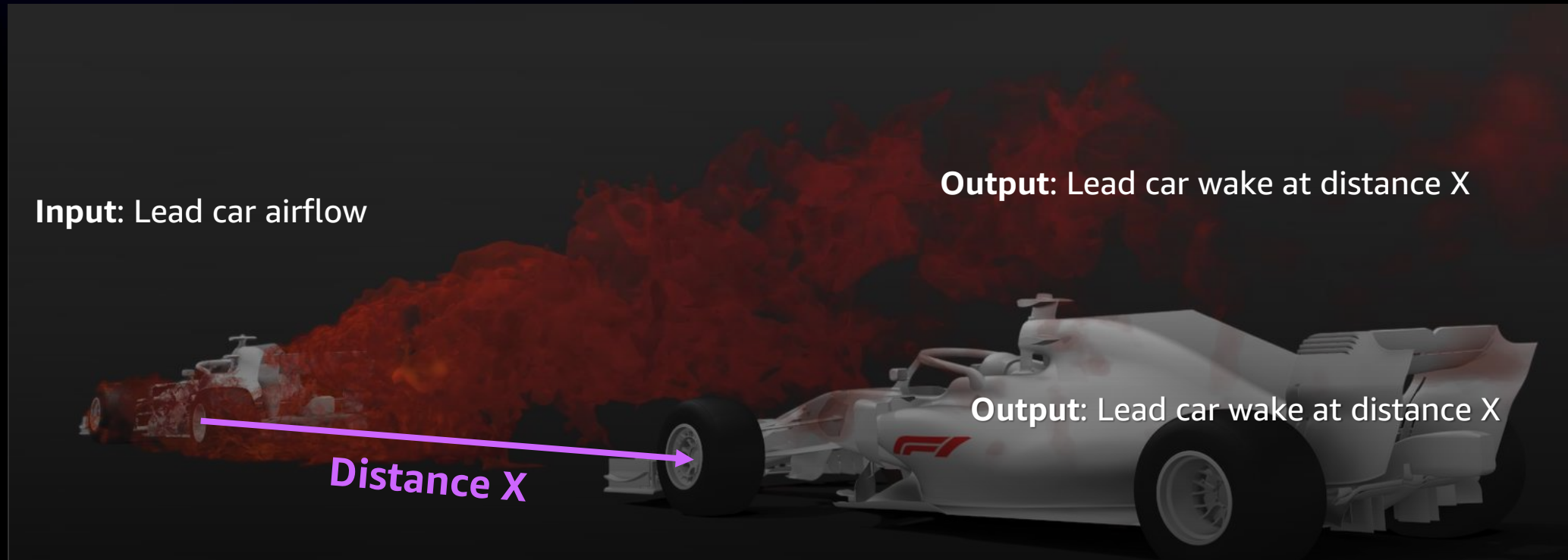


Credit: "Physics Informed Deep Learning,"
<https://maziarraissi.github.io/PINNs/>

AI-driven infrastructure optimization

Demonstrating ML + HPC

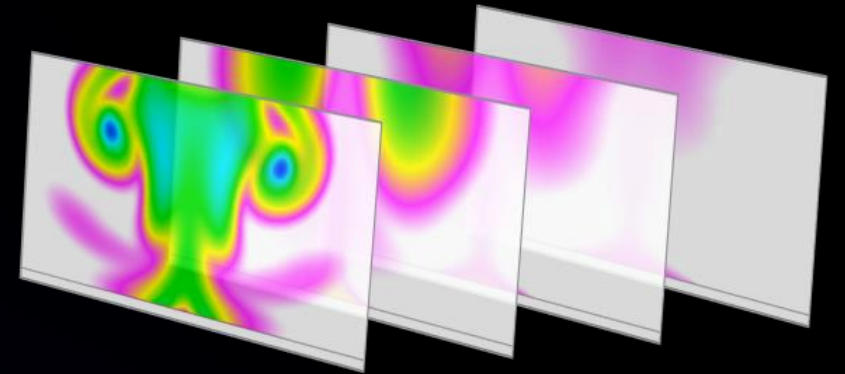
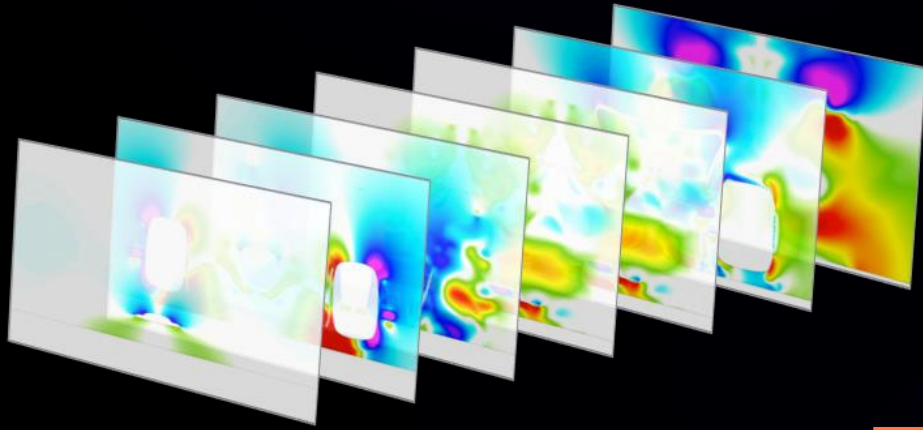
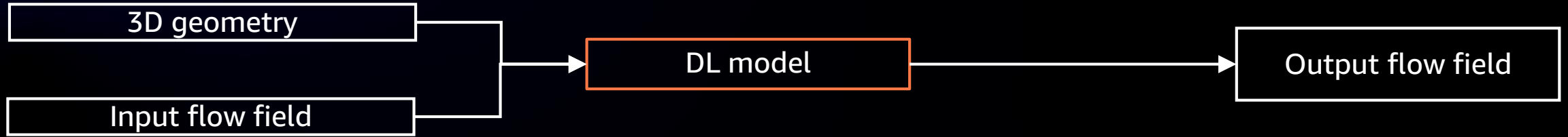
EXTRACT RELATIONSHIPS FROM HPC SIMULATION RESULTS



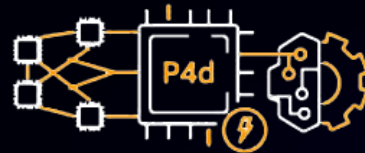
Problem statement:

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

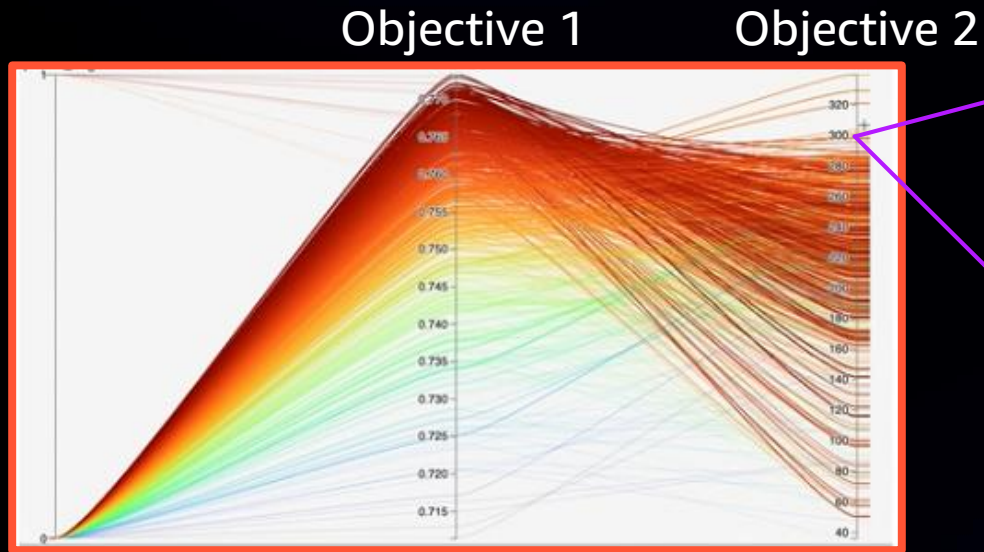
ML + HPC solution



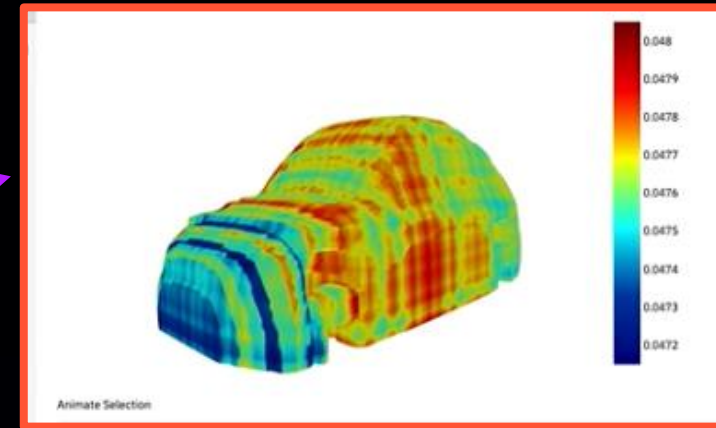
EC2 UltraClusters



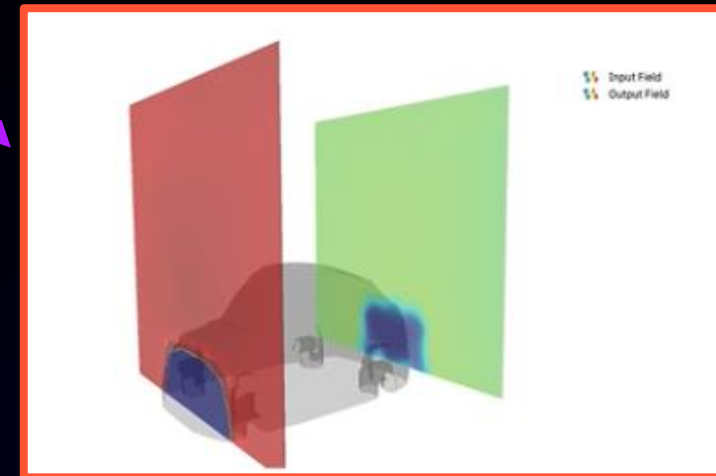
Mapping trajectories to design solutions



Optimal geometry



Optimal flow field

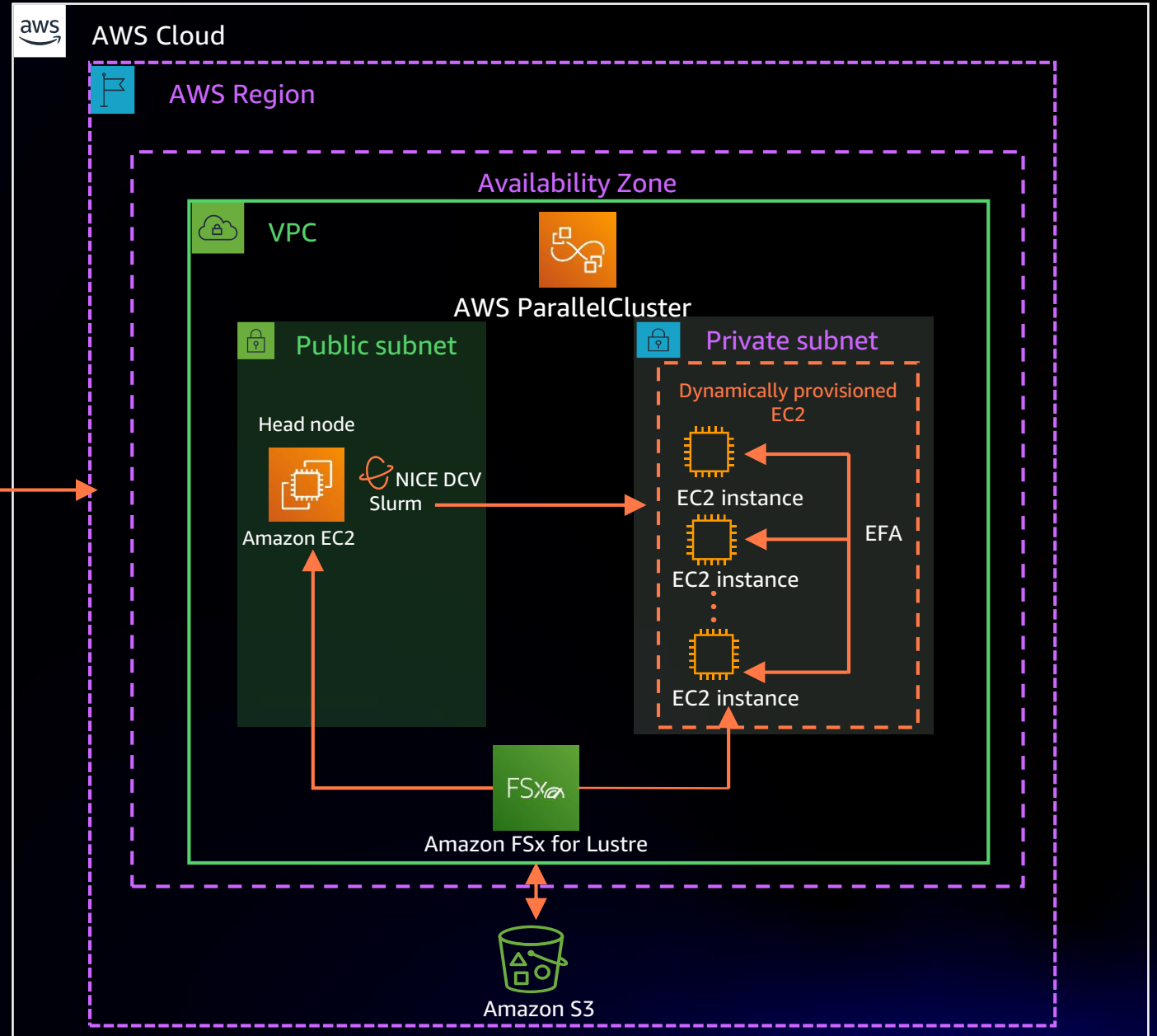
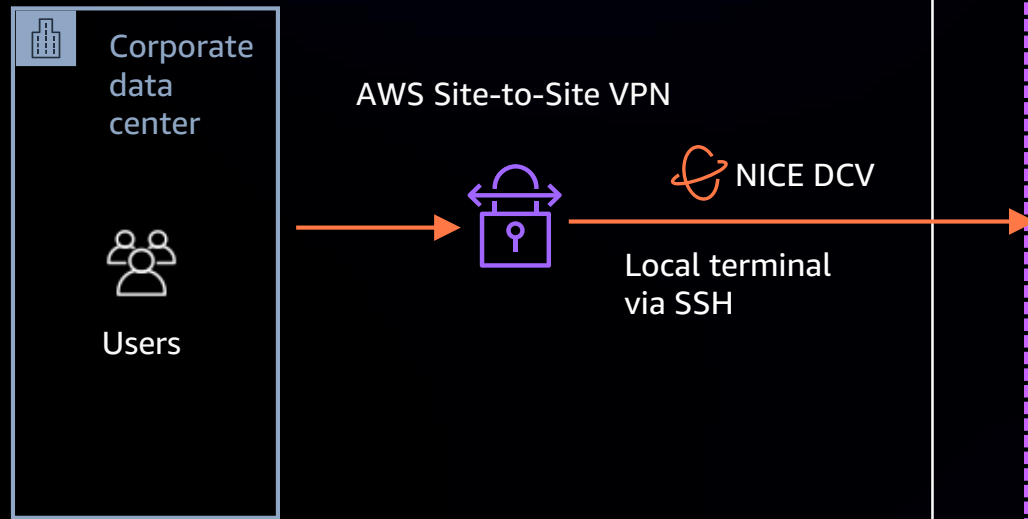


Jyothi Venkatesh

Specialist HPC Solutions Architect, AWS



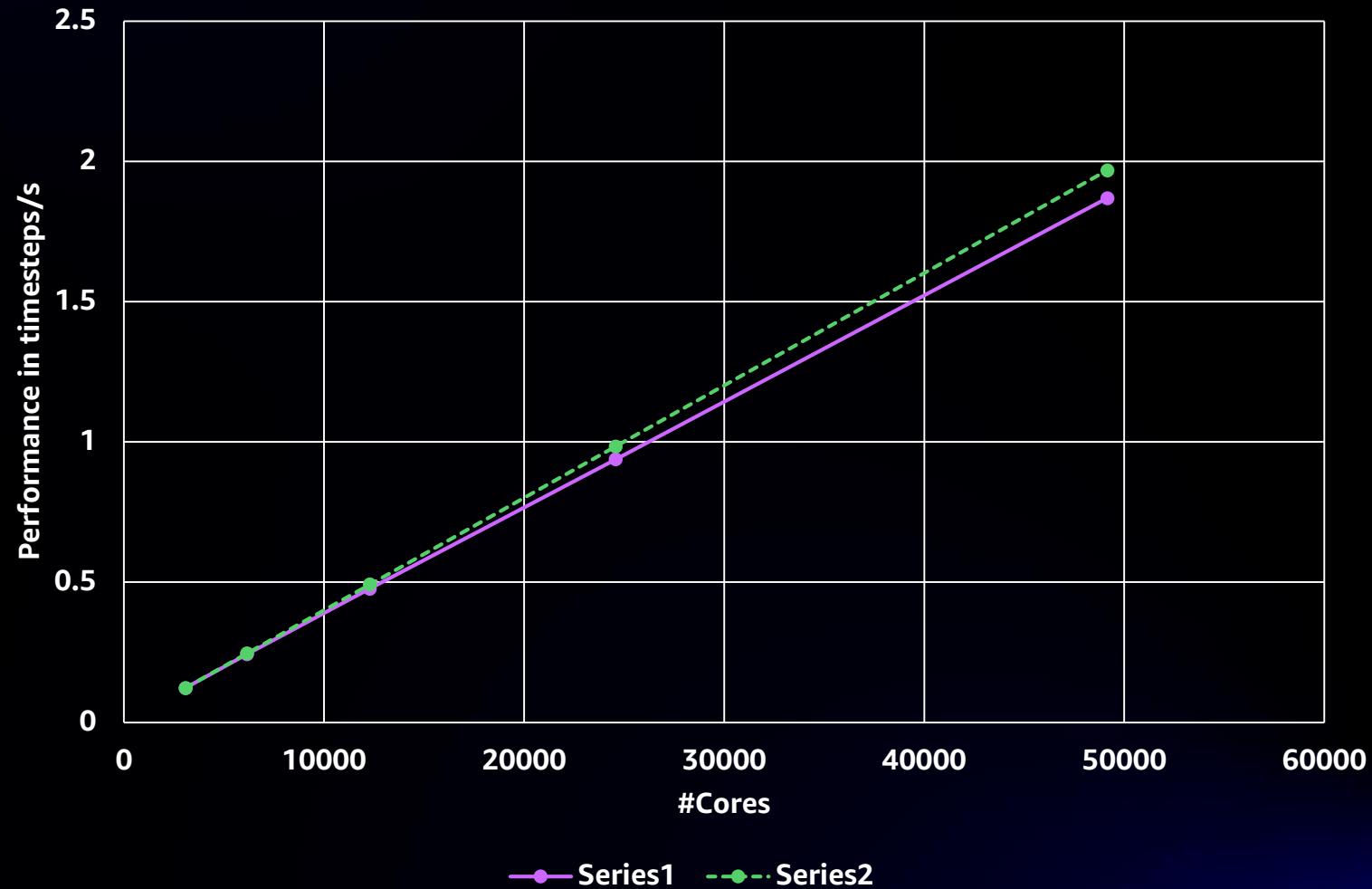
HPC architecture



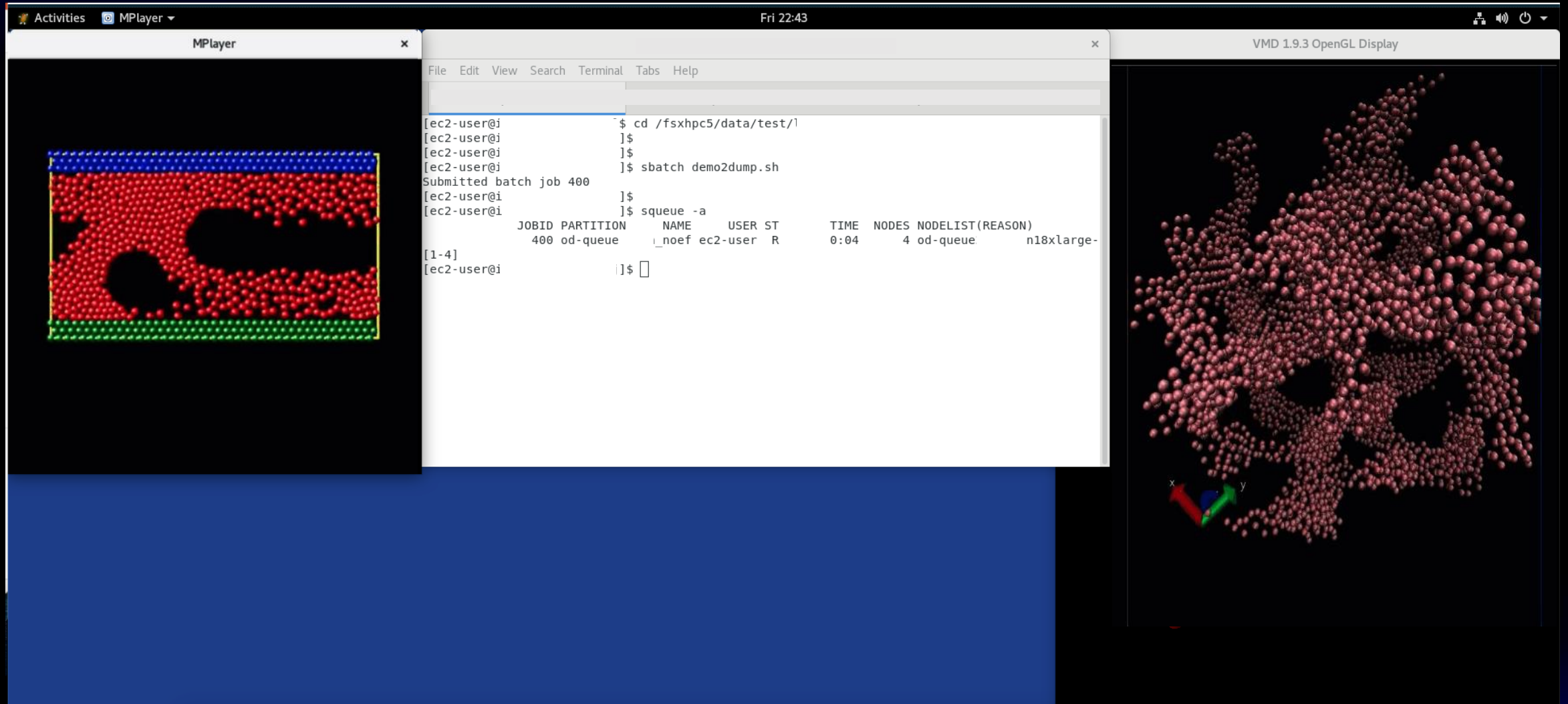
Scaling LAMMPS on AWS



Scaling LAMMPS on Amazon EC2 with EFA: 27B atoms



Running HPC applications on AWS



The screenshot displays a desktop environment with three windows open:

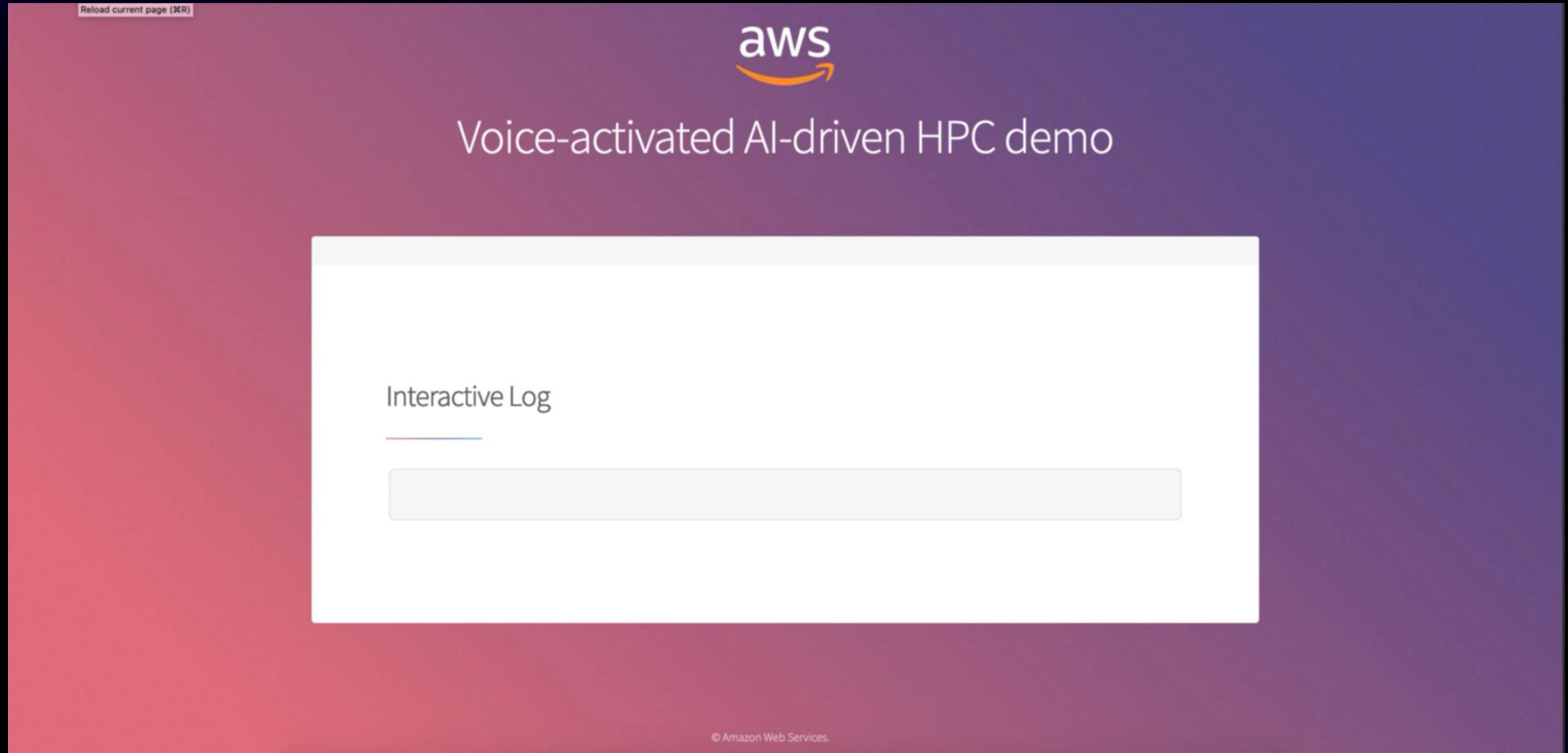
- MPlayer:** A window showing a 2D visualization of a molecular simulation. It features a central region of red spheres with two black circular voids, surrounded by a layer of blue spheres at the top and a layer of green spheres at the bottom.
- Terminal:** A window showing a shell prompt and several commands being executed. The output includes a table of job information.
- VMD 1.9.3 OpenGL Display:** A window showing a 3D visualization of a molecular simulation. It displays a large, dense cluster of red spheres, with a small 3D coordinate system (x, y, z) visible in the bottom left corner.

```
[ec2-user@i]$ cd /fsxhpc5/data/test/1
[ec2-user@i]$ 
[ec2-user@i]$ 
[ec2-user@i]$ sbatch demo2dump.sh
Submitted batch job 400
[ec2-user@i]$ 
[ec2-user@i]$ squeue -a
```

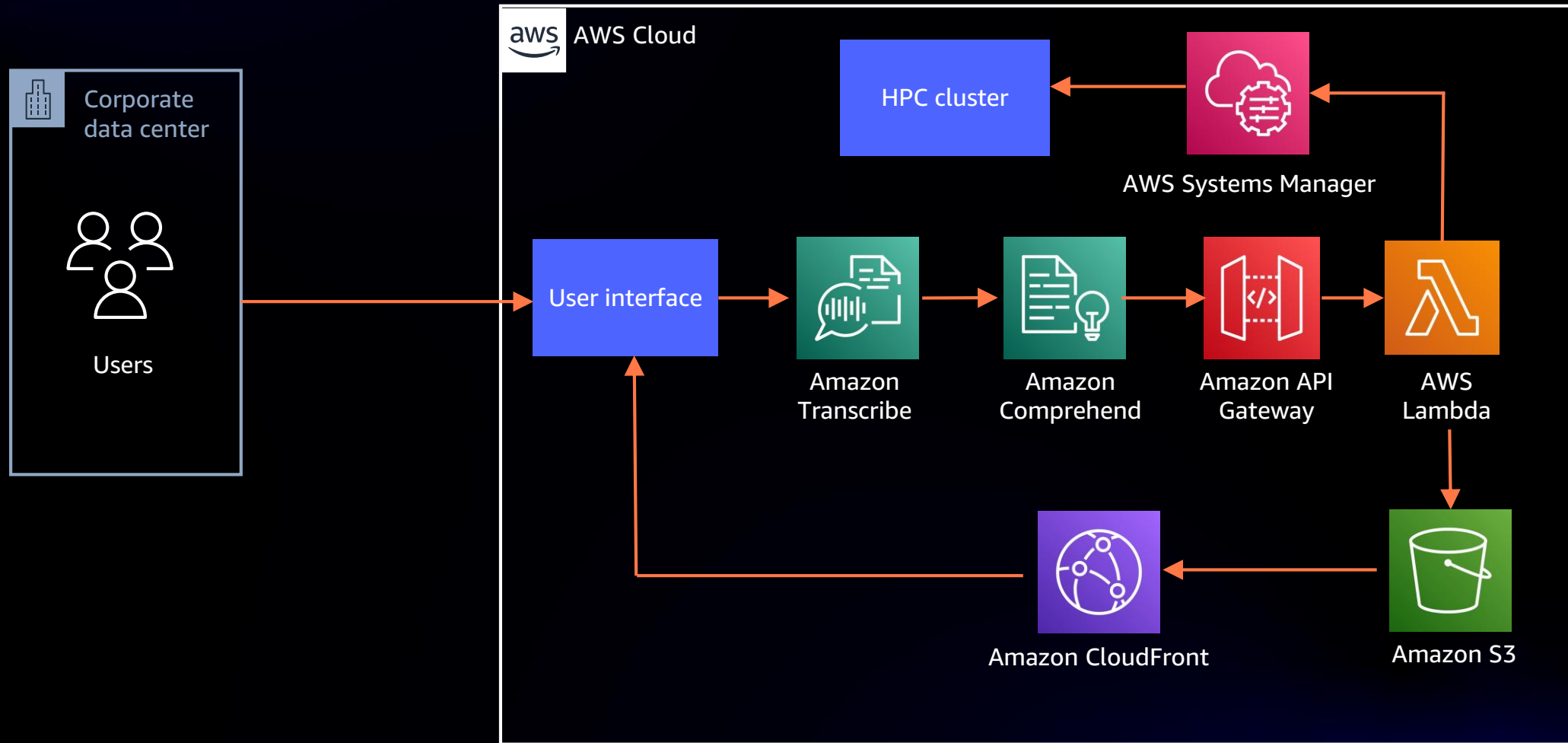
JOBID	PARTITION	NAME	USER	ST	TIME	NODES	MODELIST(REASON)
400	od-queue	_noef	ec2-user	R	0:04	4	od-queue n18xlarge-

```
[1-4]
[ec2-user@i]$
```

AI-driven HPC: The future is here!



Voice-activated, AI-driven HPC demo



AWS and Descartes Labs: Planetary-scale modeling for sustainability



Jeff Barr blog: <https://aws.amazon.com/blogs/aws/planetary-scale-computing-9-95-pflops-position-41-on-the-top500-list/>

Note: Descartes Labs moved up from #41 to #40 after official rankings were announced due to the removal of the #33 entry



THE FUTURE OF HPC IS LOOKING A LOT LIKE ML

Going beyond net zero commitments

Terry Cunningham (he/him)
Descartes Labs
CEO

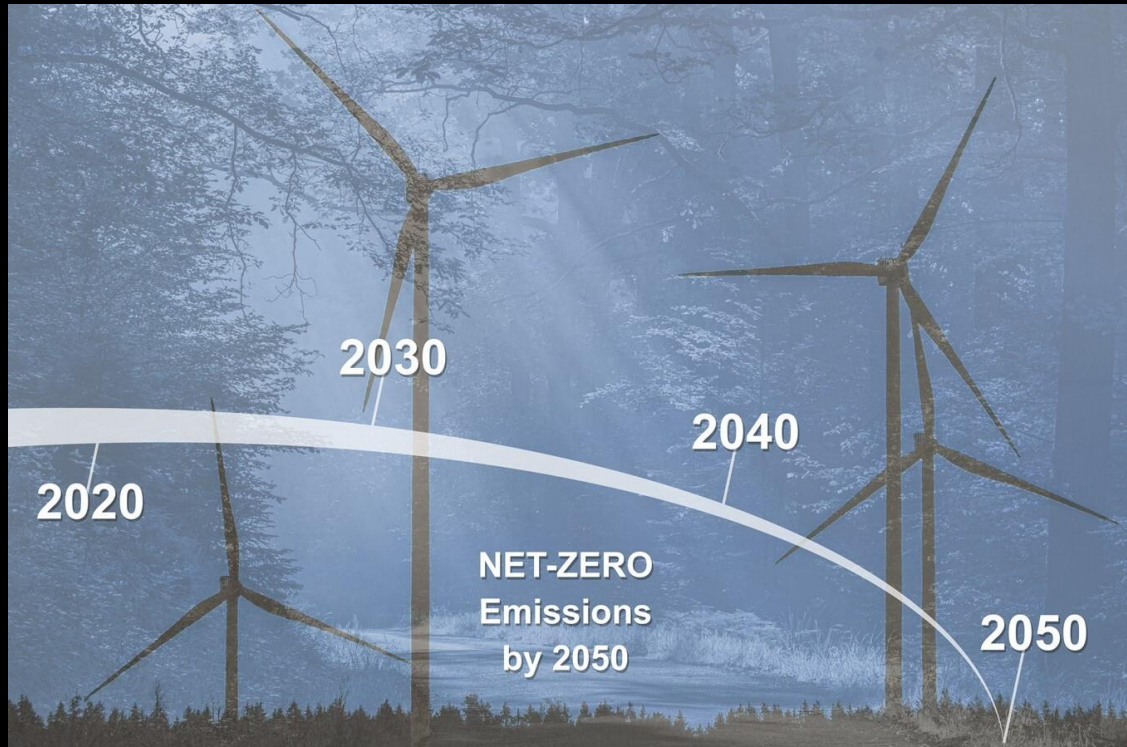




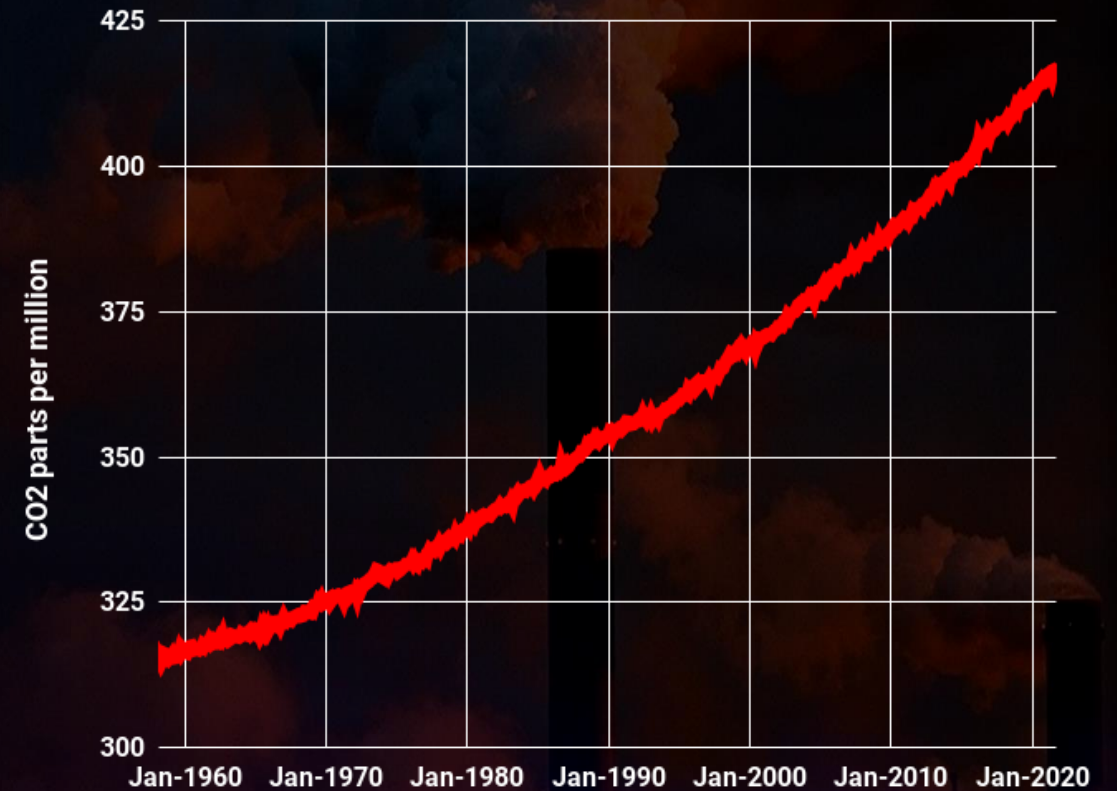
Net zero commitments

HOW IT STARTED

Hundreds of companies pledge to achieve net zero emissions



HOW IT'S GOING



For good, measure!

THERE IS NO 1.5°C WORLD WITHOUT
TRANSFORMING THE LAND-USE ECONOMY

25%

of global emissions
are from land use

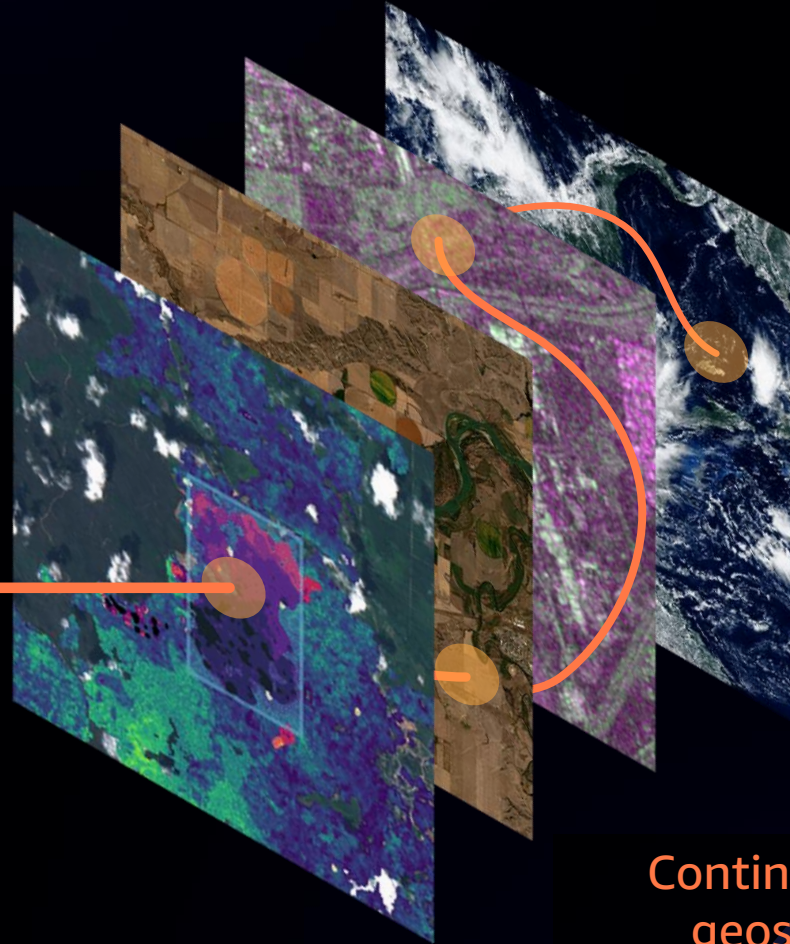




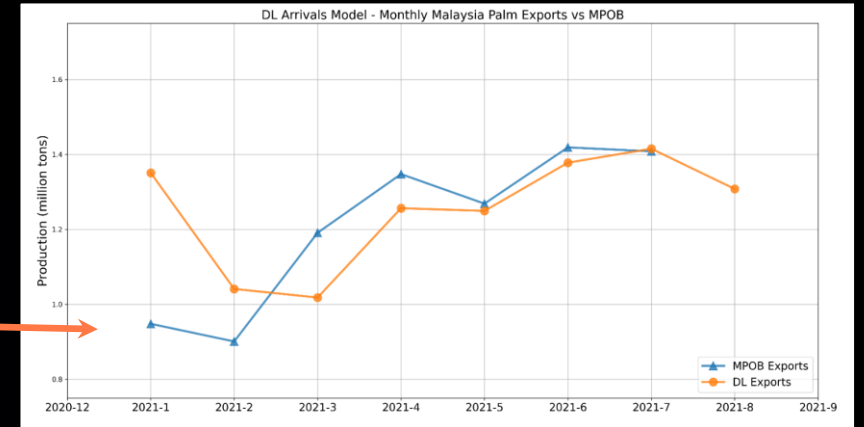
**How do we pay
for sustainability?**

For profit, forecast!

HPC with AWS



Smart procurement with improved price forecasts



Continuously updating geospatial insights



Price forecasts can help fund sustainability initiatives



+



Descartes
Labs



FORECASTING

4% savings

using a more accurate
palm price forecast



SUSTAINABILITY

Deforestation alerts

of particular salience and importance

Funds

AWS News Blog

Planetary-Scale Computing – 9.95 PFLOPS & Position 40 on the TOP500 List

by Jeff Barr | on 28 JUN 2021 | in [Amazon EC2](#), [High Performance Computing](#), [Launch](#), [News](#) | [Permalink](#) | [Comments](#) | [Share](#)



Amazon EC2 Instance Cluster us-east-1a - Amazon EC2 r5.24xlarge,
Xeon Platinum 8260 24C 2.4GHz, 25G Ethernet

Descartes Labs, United States

is ranked

No. 40

among the World's TOP500 Supercomputers

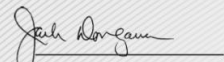
with 9.95 PFlop/s Linpack Performance

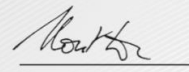
in the 57th TOP500 List published at the ISC Virtual 2021

Conference on June 28, 2021.

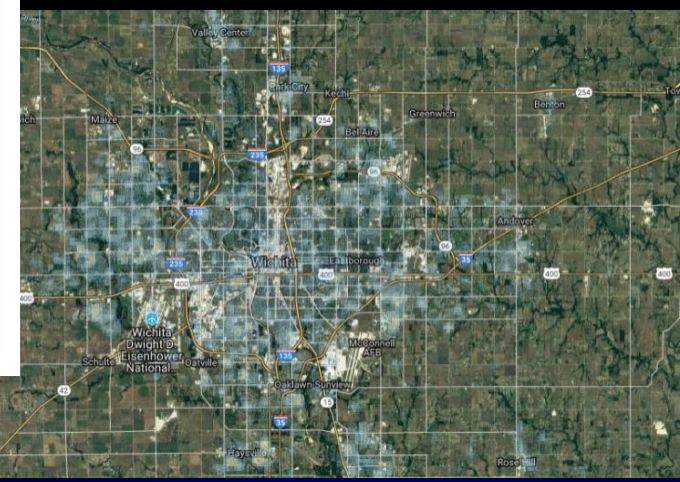
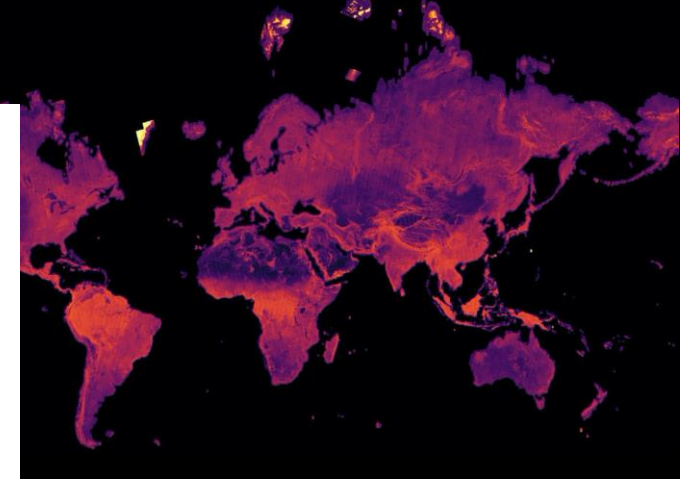
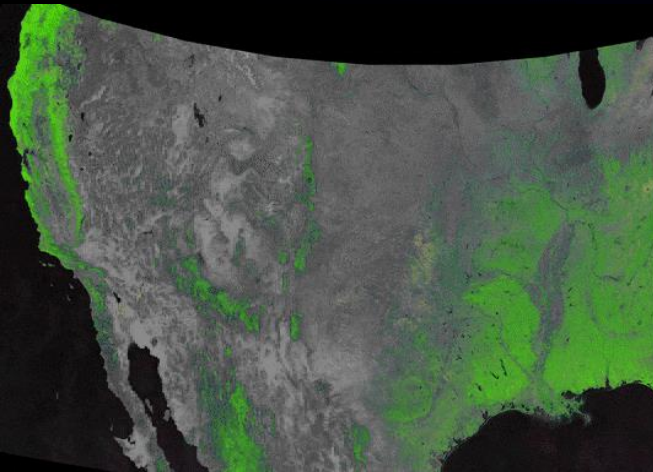
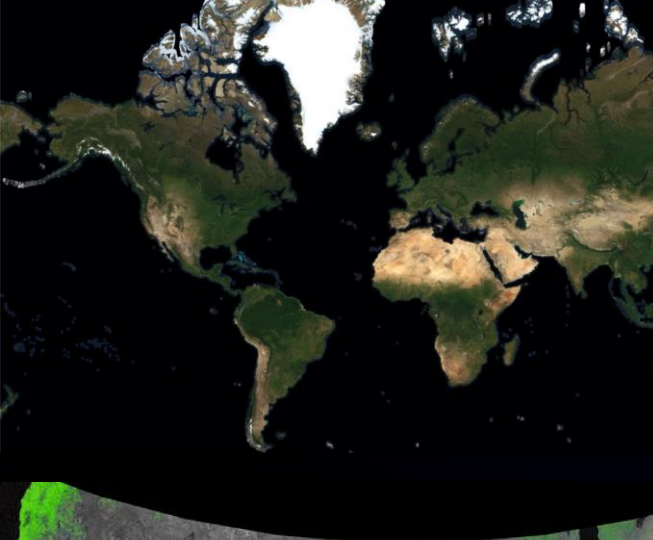
Congratulations from the TOP500 Editors


Erich Strohmaier
NERSC/Berkeley Lab


Jack Dongarra
University of Tennessee


Horst Simon
NERSC/Berkeley Lab


Martin Meuer
Prometheus



This is only possible with AWS

Storage

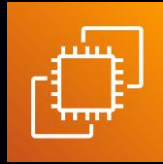


Amazon Simple Storage Service (Amazon S3)



Amazon S3 Storage Lens

Compute



Amazon Elastic Compute Cloud (Amazon EC2)

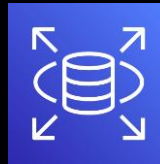


AWS Lambda



AWS Batch

Database

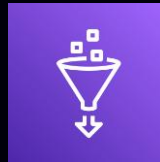


Amazon Relational Database Service (Amazon RDS)

Analytics



Amazon Redshift



AWS Glue

Containers



Amazon Elastic Kubernetes Service (Amazon EKS)



Amazon Elastic Container Service (Amazon ECS)

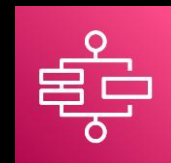


AWS Fargate

Integration



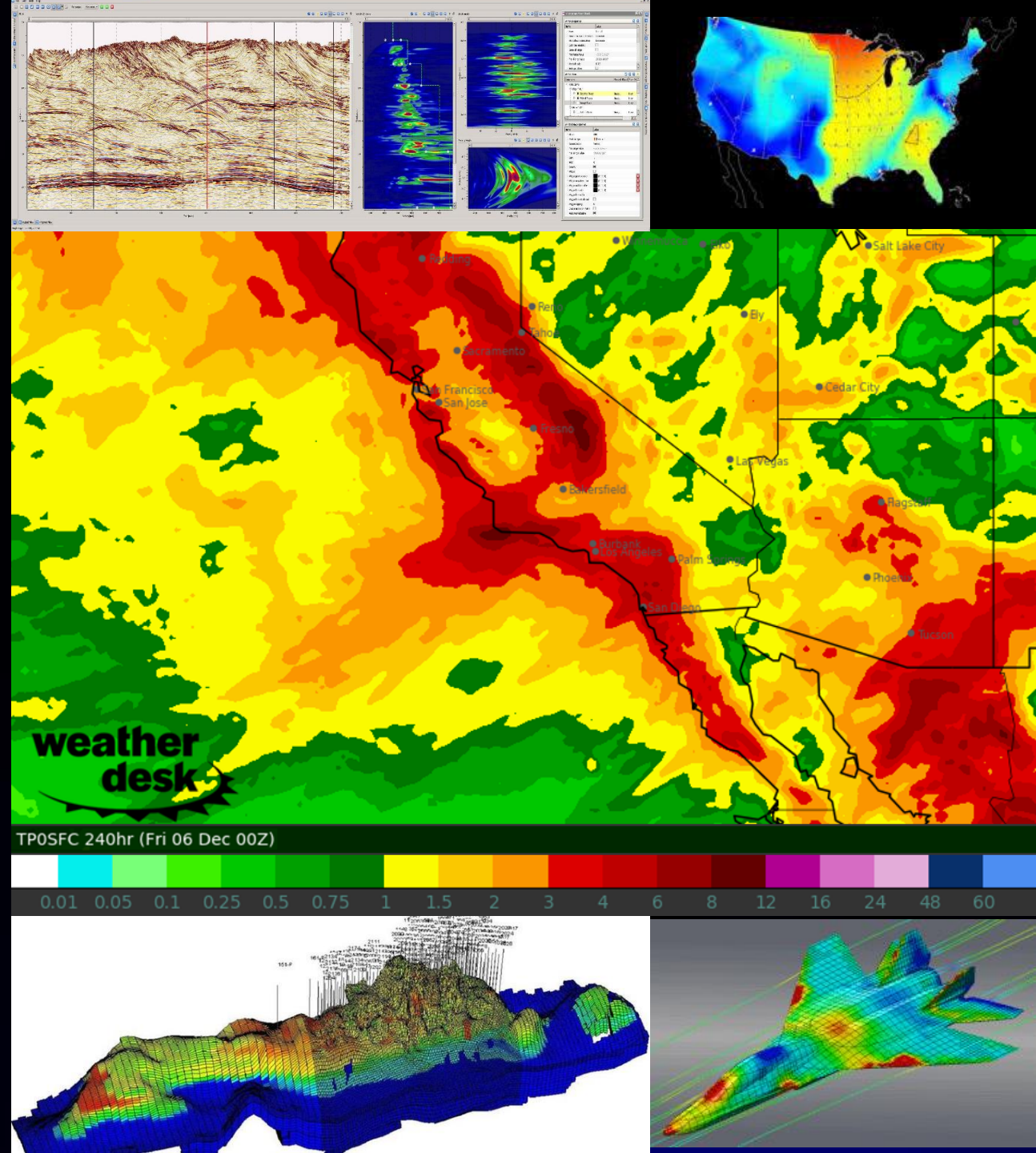
Amazon Simple Queue Service (Amazon SQS)



AWS Step Functions

HPC + ML on AWS enables customers to find new business value

Rethink . . .
Reinvent . . .
Results . . .



Thank you!