AWS re:Invent

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CMP318

Accelerating the drug discovery pipeline

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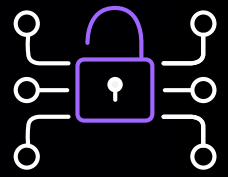
Emerging challenges and trends in R&D

Computational chemistry and structural biology

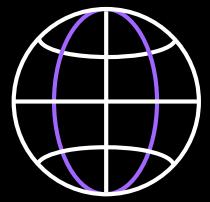
Modeling and simulation

Imaging

Genomics



Compliant and secure environment



Global, fault-tolerant infrastructure

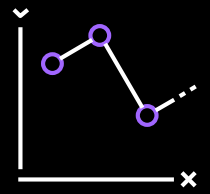
Data science

High throughput computing

High performance computing



Accelerated time to insight



Scalability and dynamic resourcing

Innovation and partnership ⟷ User experience ⟷ Operational excellence

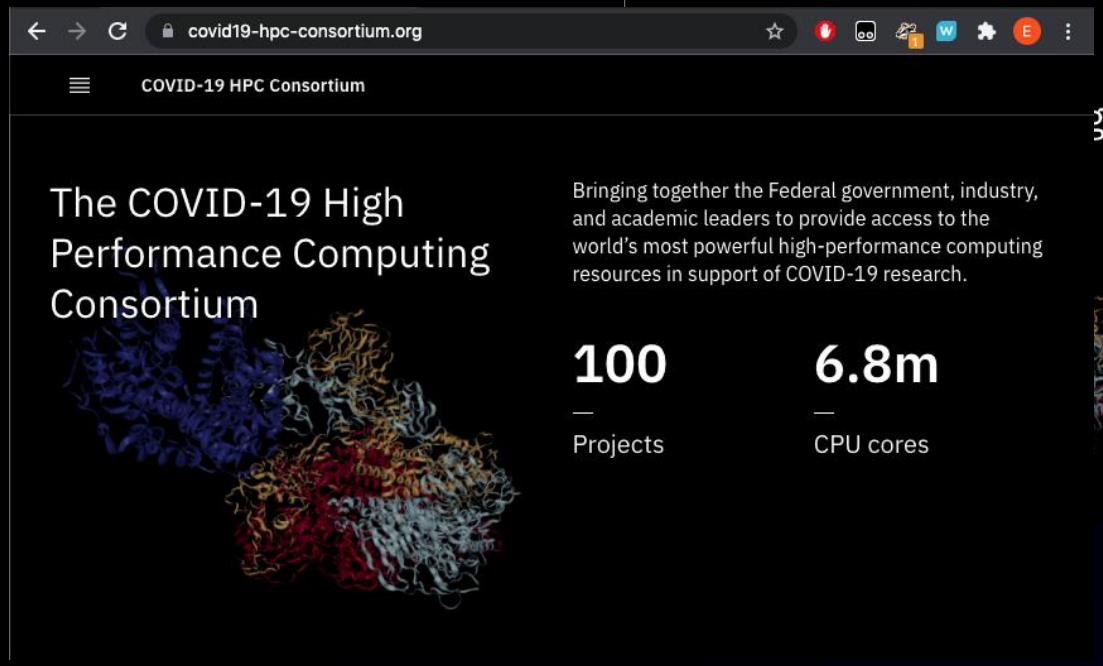
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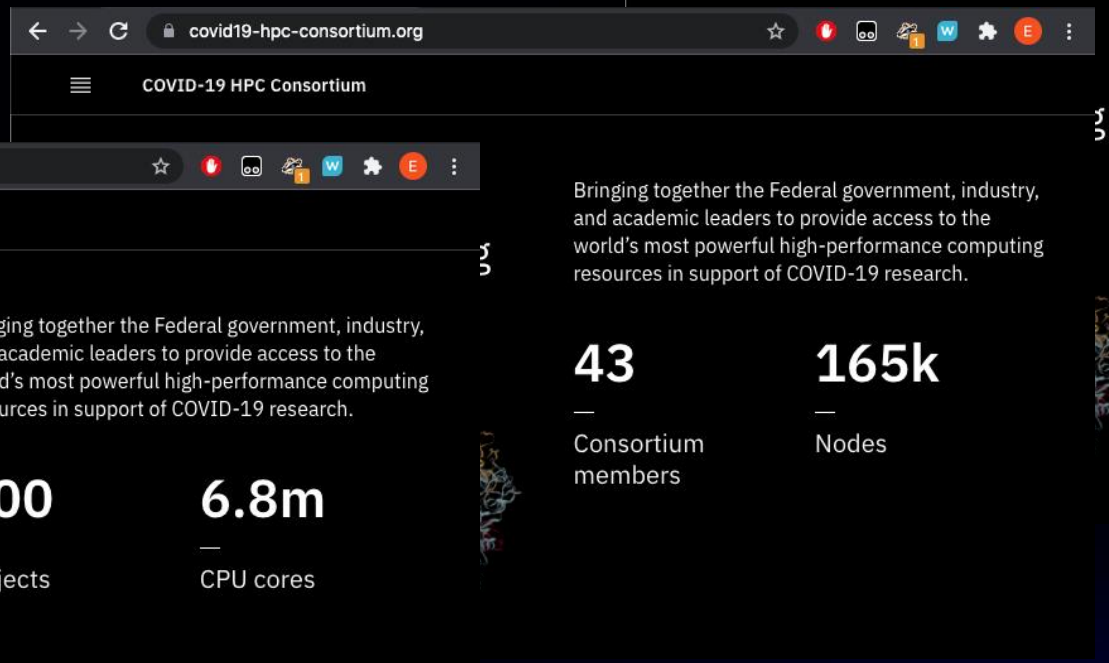
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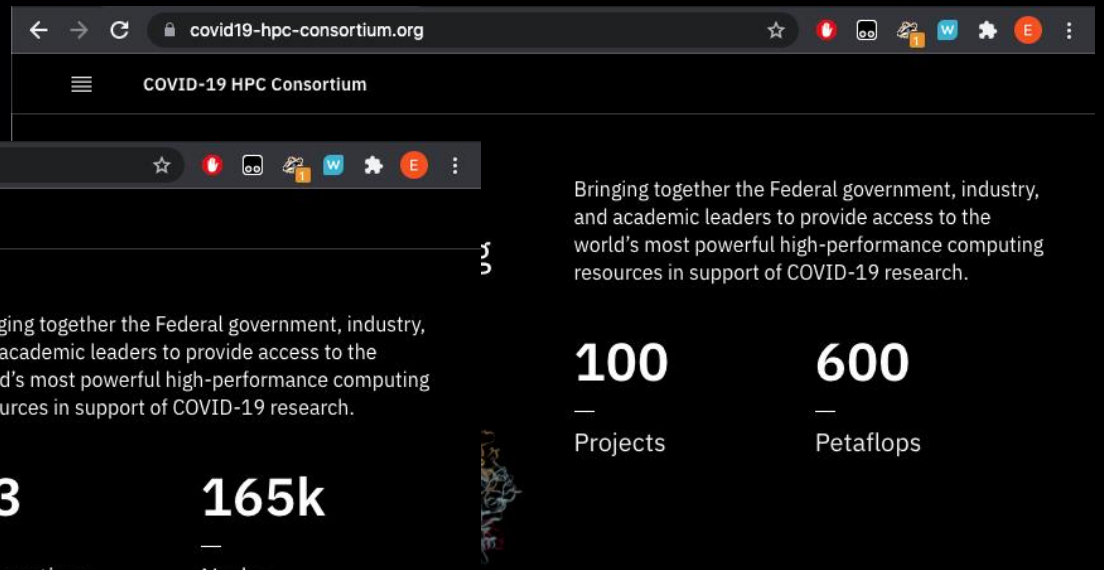
COVID-19 HPC consortium

"Working together, government, business, and academic leaders can utilize the power of the cloud to advance the pace of scientific discovery and innovation, and help combat the COVID-19 virus."

Teresa Carlson
Former VP
WWPS (AWS)

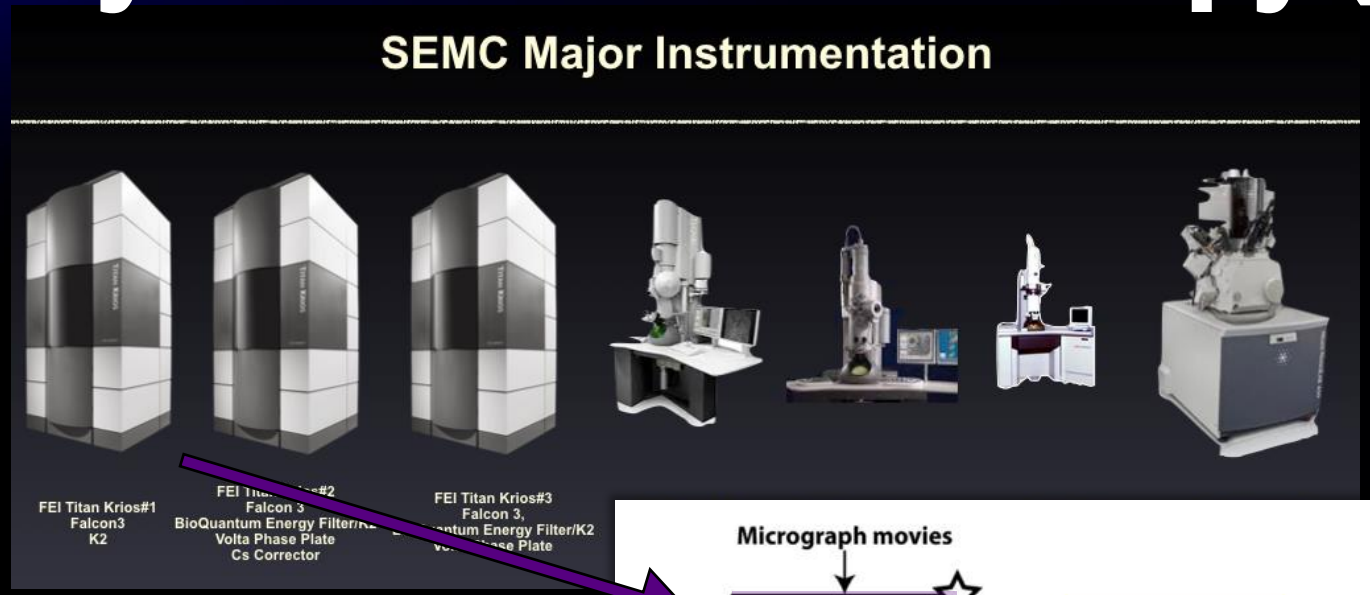




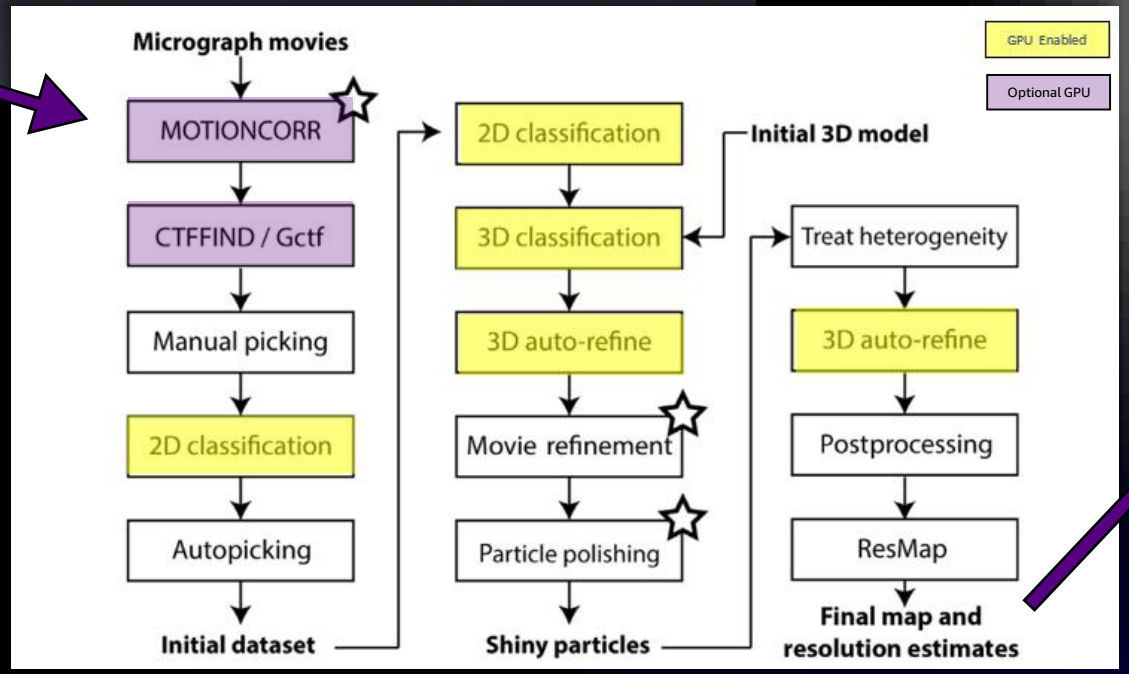


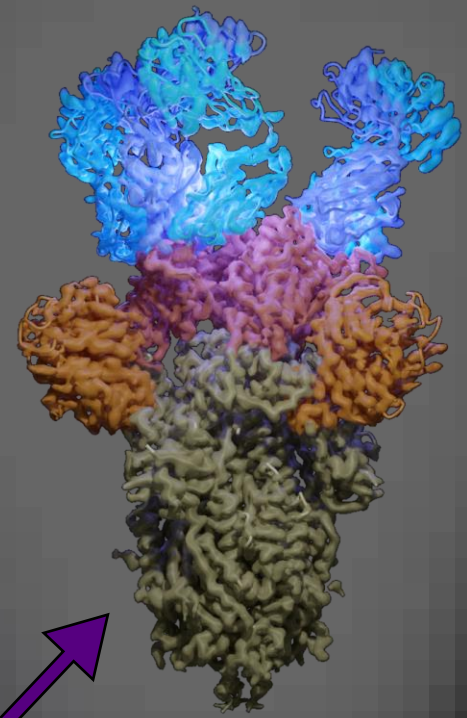
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Cryo-electron microscopy (cryo-EM)



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



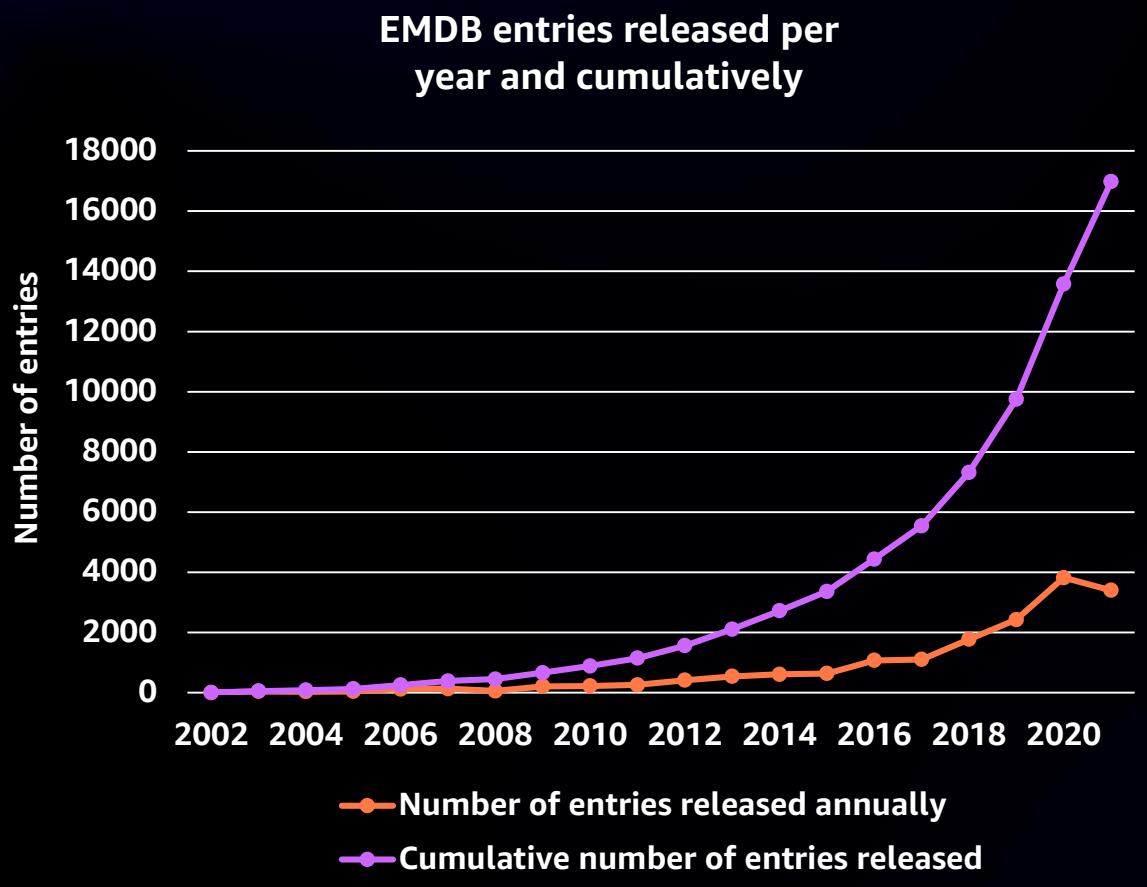


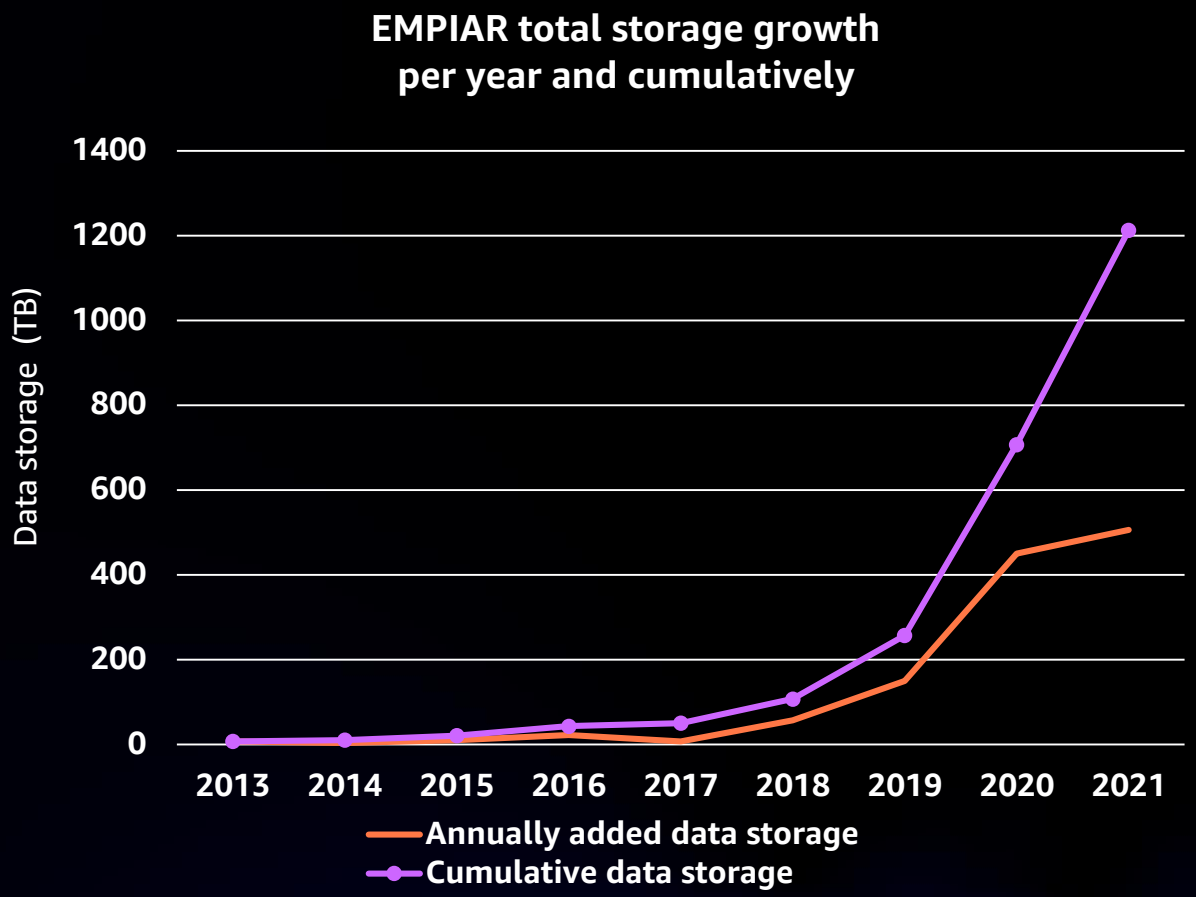
Antibody 2-4
Liu et al., *Nature* 2020
PDB 6XEY
10.1038/s41586-020-2571-7
Structure courtesy of Micah Rapp

https://aws.amazon.com/blogs/industries/building-a-gpu-enabled-cryoem-workflow-on-aws/

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Growth of cryo-electron microscopy





Source: Electron Microscopy Data Bank: https://www.ebi.ac.uk/emdb/statistics

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Adding elasticity and enterprise security to scientific software

Roberto Iturralde
Sr. Director, Software Engineering

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At Vertex, we strike at the core of serious diseases to change people's lives; bringing together the brightest minds, investing in science and taking smart risks, we go all in for cures; we are fueled by the needs of patients, families, doctors and nurses; their hope and courage drive us to work another day, stay another hour, sleep a little less and do a little more; for the lives we have changed and for those who are still waiting, we will never stop fighting until we discover a cure

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Scientific software often presents enterprise challenges

Lacks key security features

- Single sign-on integration (SAML/OIDC)
- LDAP integration
- Encryption in transit/TLS
- System access audit trail

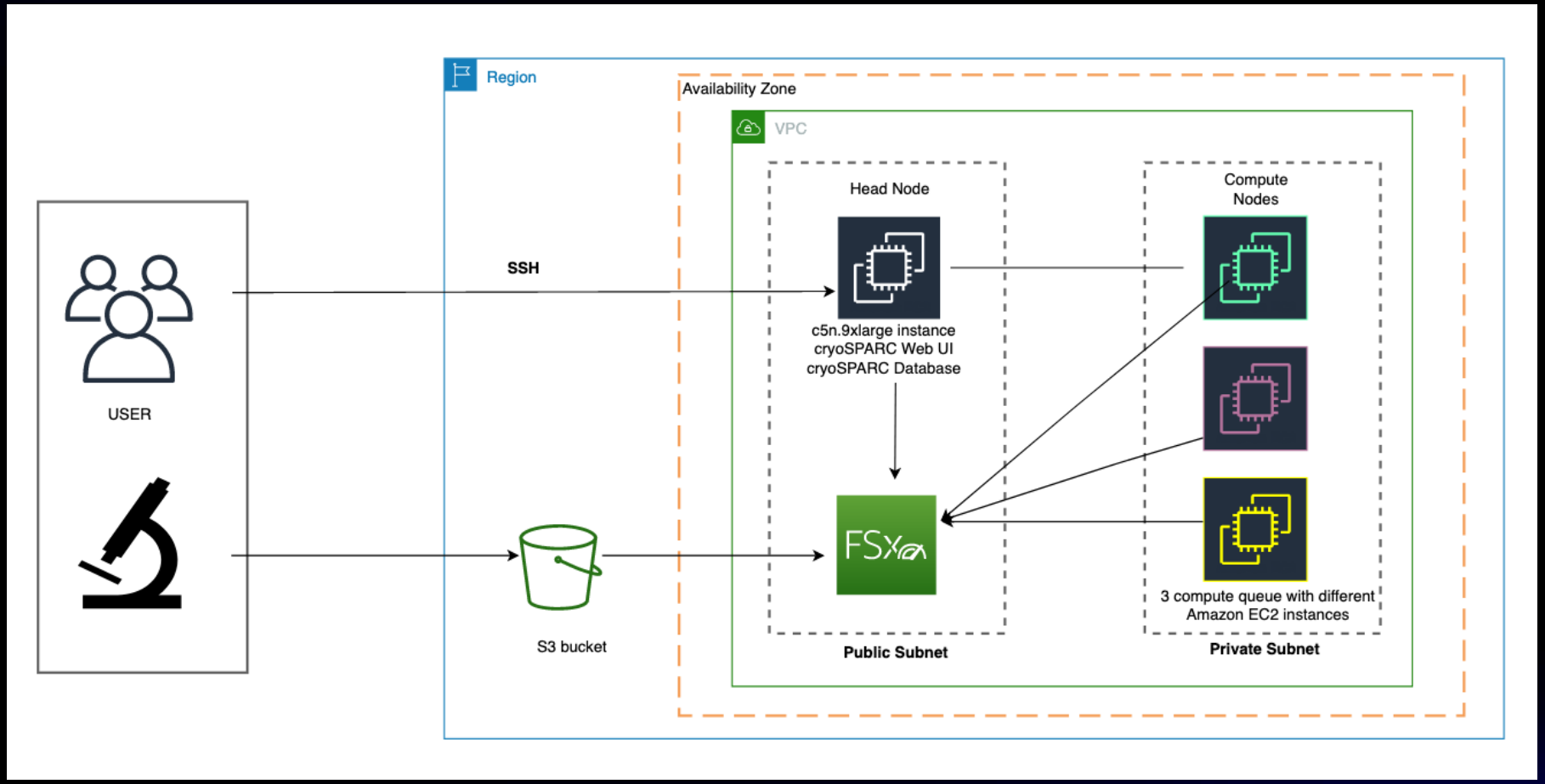
Infrastructure hungry

- Scientific instruments can generate terabytes of data daily, petabytes annually
- Scientific software can require specialized hardware (e.g., GPUs) for efficient analysis
- Software usage often aligned to phases of research pipeline; spikey demand

aws

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Example: CryoSparc – CryoEM analysis software



https://guide.cryosparc.com/deploy/cryosparc-on-aws

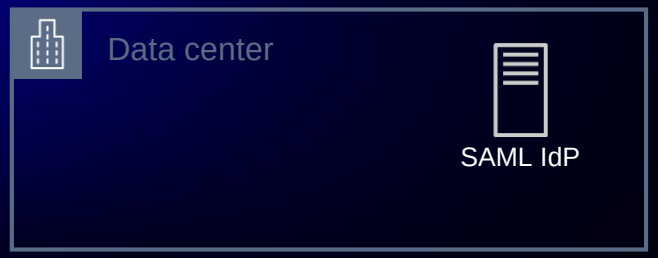
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Architecture

- Amazon EC2 instances for head and compute
- Amazon FSx Lustre for high-performance file system
- Scientists access environment by private IP address over HTTP

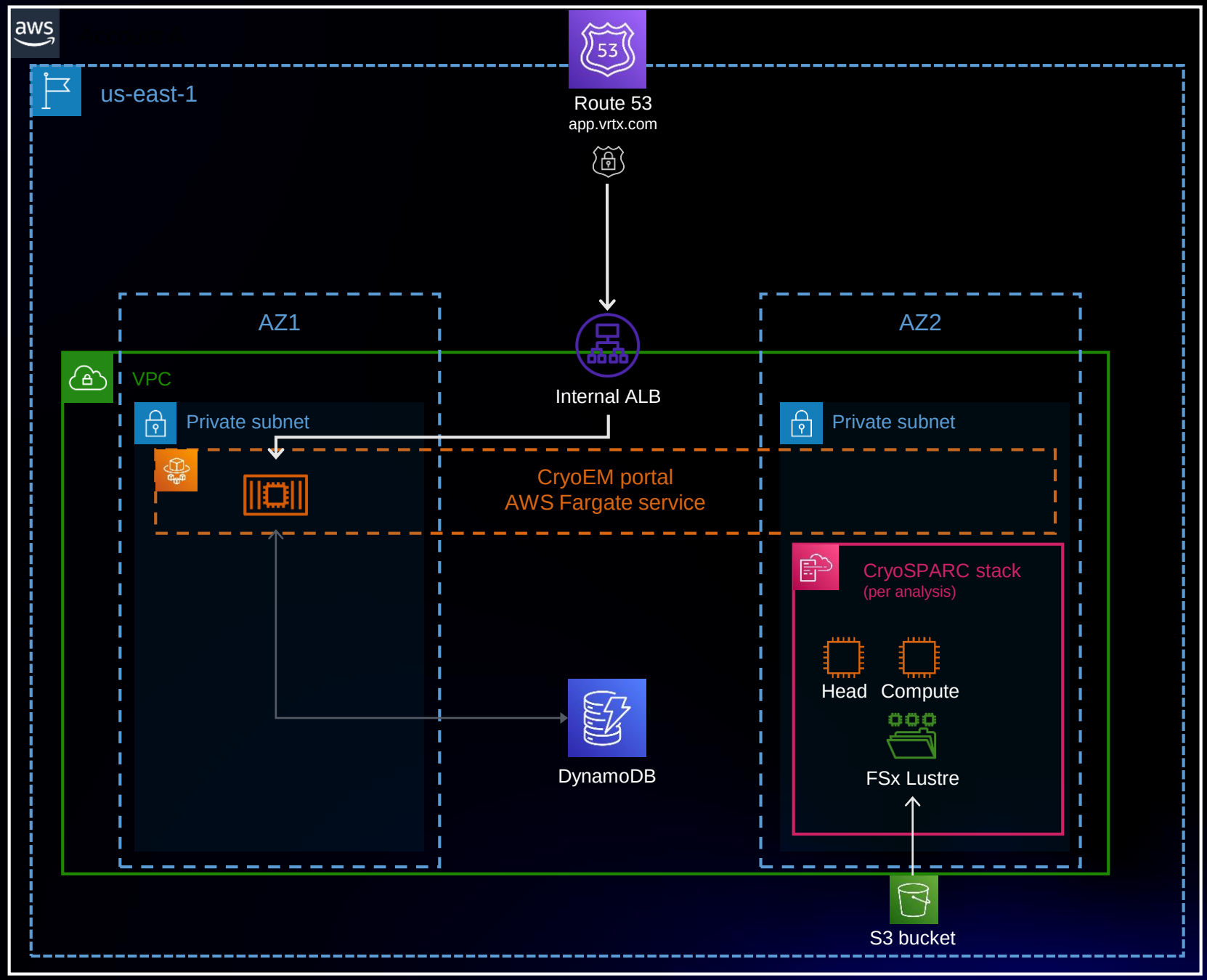


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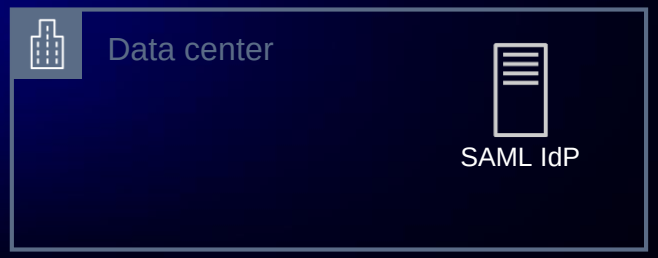


Improvements

- Store CryoEM data in Amazon S3; load into FSx for analysis and write new data back to S3
- Create a web portal that allows scientists to create CryoSparc environments on-demand
- Create AWS CloudFormation template to standardize creation of CryoSparc environments
- Create friendly DNS name in Amazon Route 53 for portal for better usability for scientists



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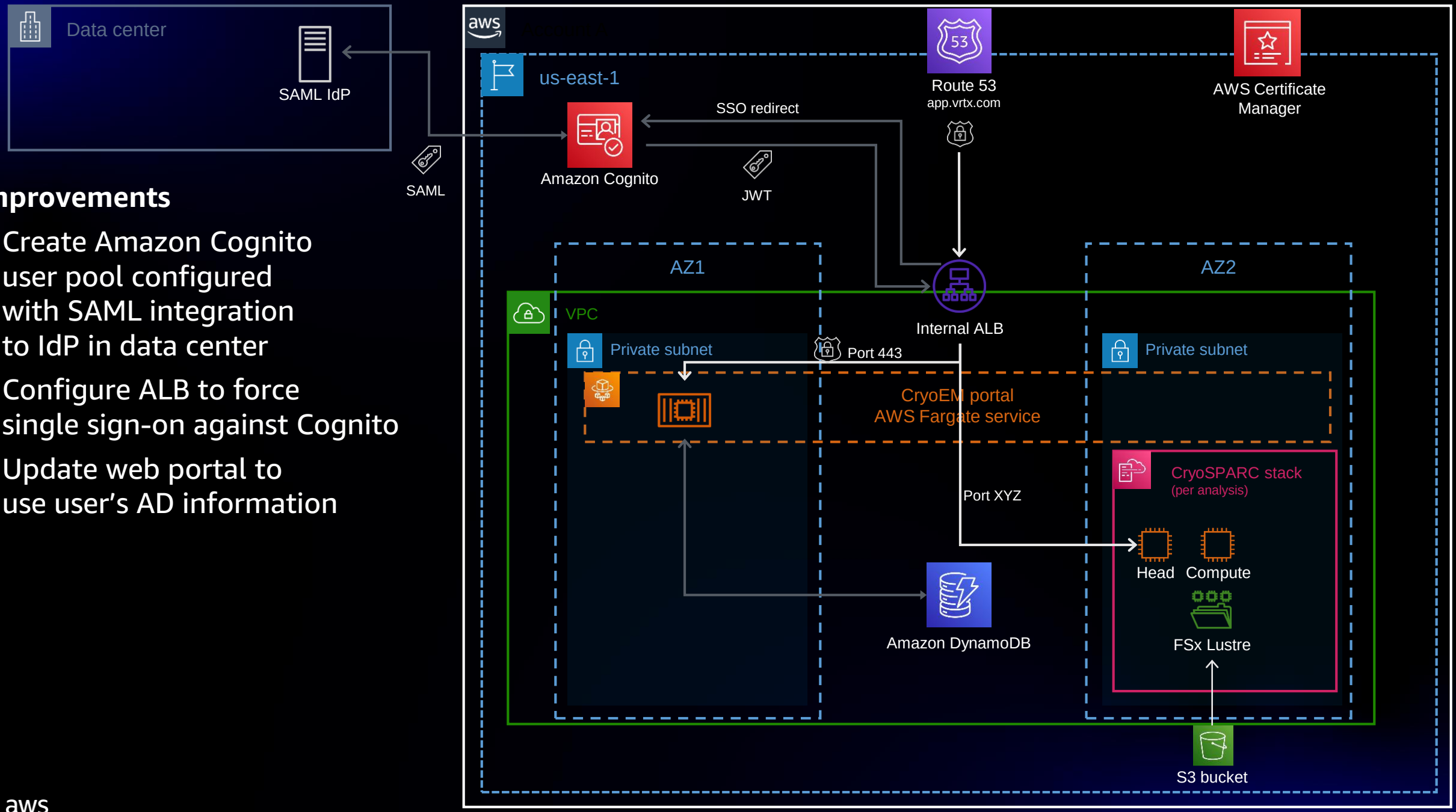
Improvements

- Register vertex certificate in AWS Certificate Manager
- Configure ALB for HTTPS; redirect HTTP to HTTPS

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Improvements

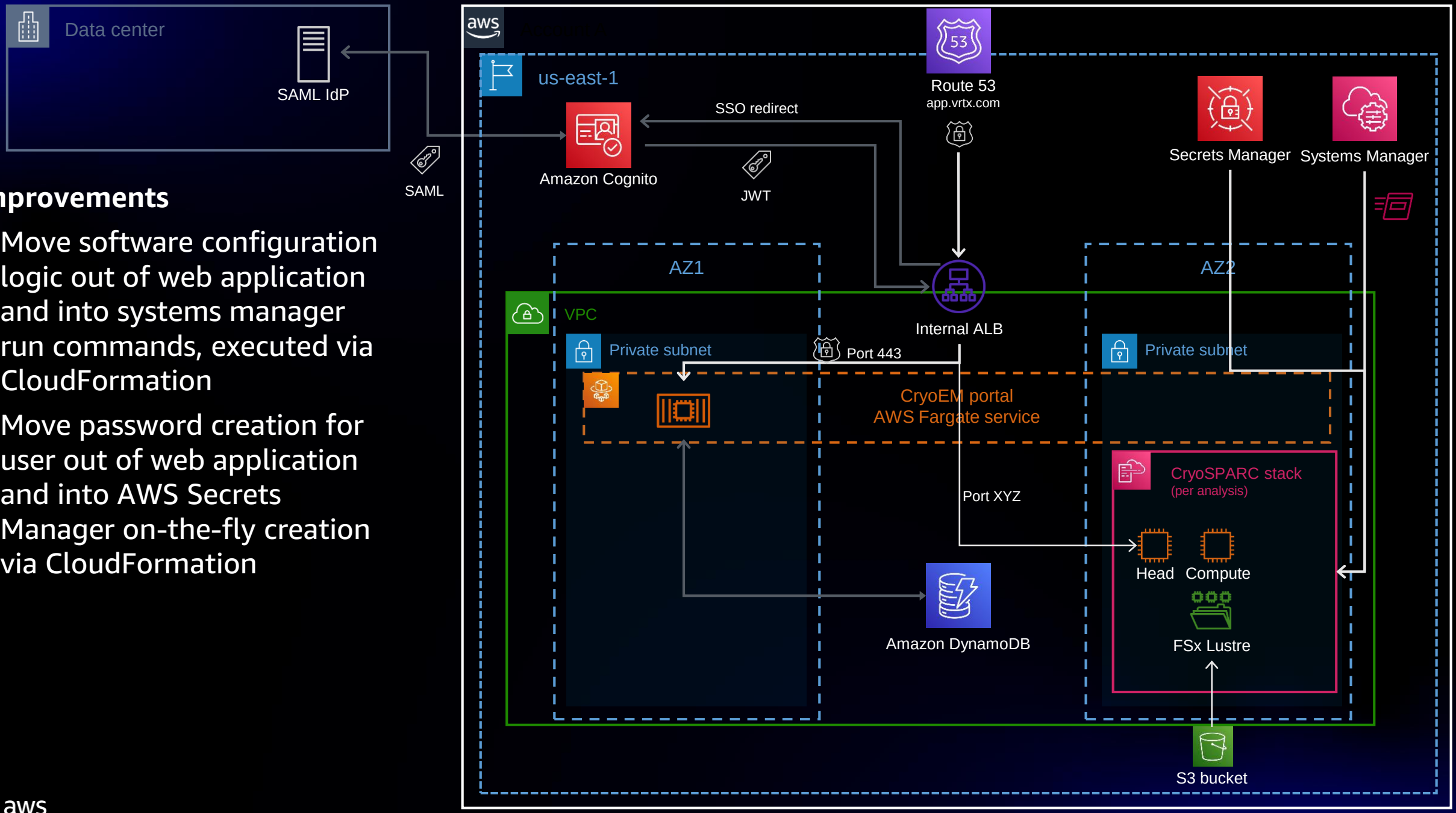
- Create Amazon Cognito user pool configured with SAML integration to IdP in data center
- Configure ALB to force single sign-on against Cognito
- Update web portal to use user's AD information



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Improvements

- Move software configuration logic out of web application and into systems manager run commands, executed via CloudFormation
- Move password creation for user out of web application and into AWS Secrets Manager on-the-fly creation via CloudFormation



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