AWS-RoseTTAFold

Brian Loyal
Sr. AI/ML Solutions Architect – Global Life Science
bloyal@amazon.com
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Session 1: What are the advantages of moving to the cloud?

Agility	Teams can experiment and innovate more quickly and frequently
Cost Savings	Only pay for what you use, lower upfront expenses
Elasticity	Easily Scale up or down with the needs of the business
Innovate Faster	Ability to focus on business differentiators, not infrastructure
Go Global in Minutes	Most extensive, reliable, and secure global cloud infrastructure

Session 2: What problems are we trying to solve?

Octank Bio needs…

To predict the structure of proteins associated with human cancers to screen against potential therapeutics.

The users of this workload…

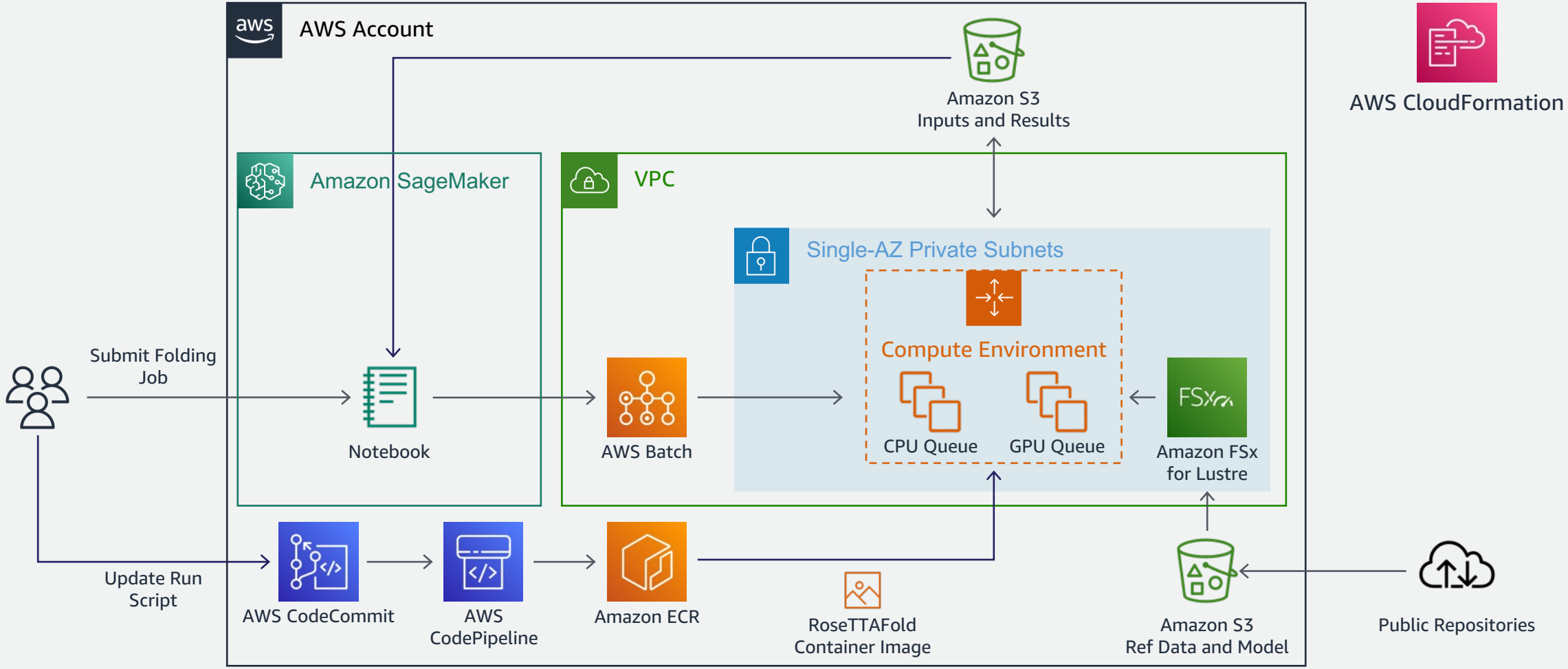
- Include ~ 30 scientists with diverse experience with high-performance computing (HPC) and bioinformatics.
- Have experience with Python programming in Jupyter notebooks
- Need to setup and (eventually) extend this workload without relying on IT

Additional requirements include…

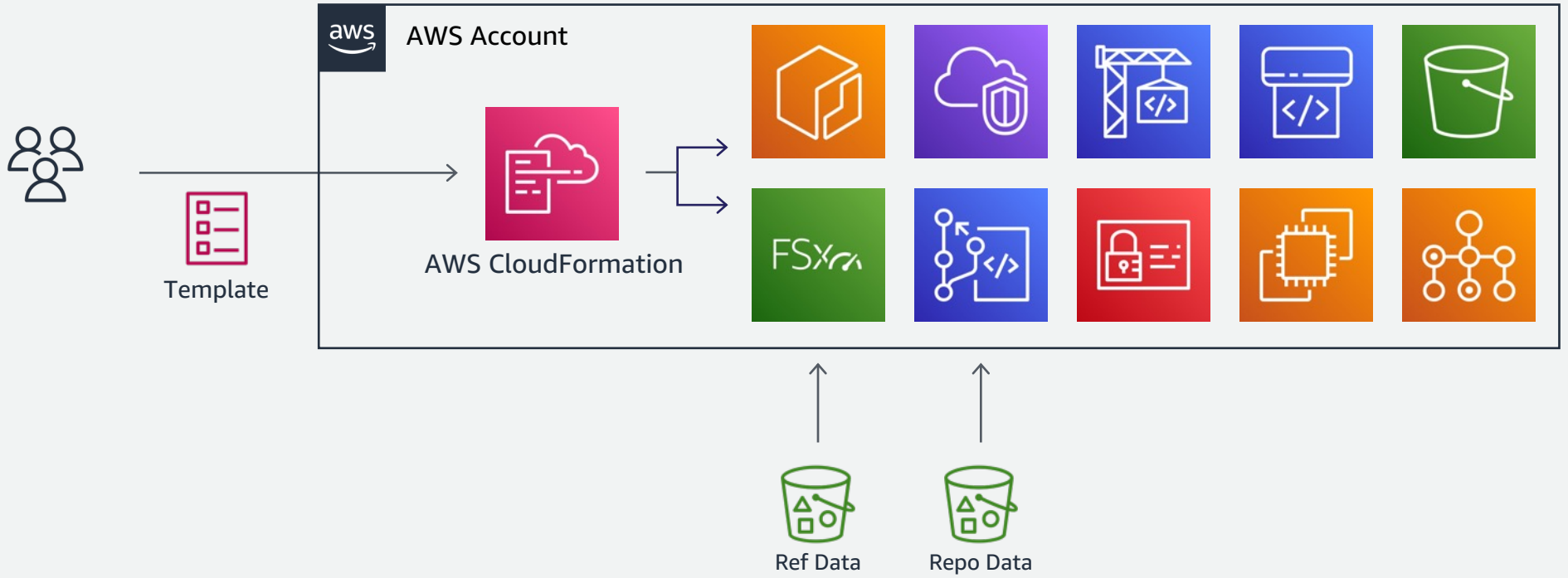
- Workload must support occasional “spikes” in activity

Demo: AWS-RoseTTAFold

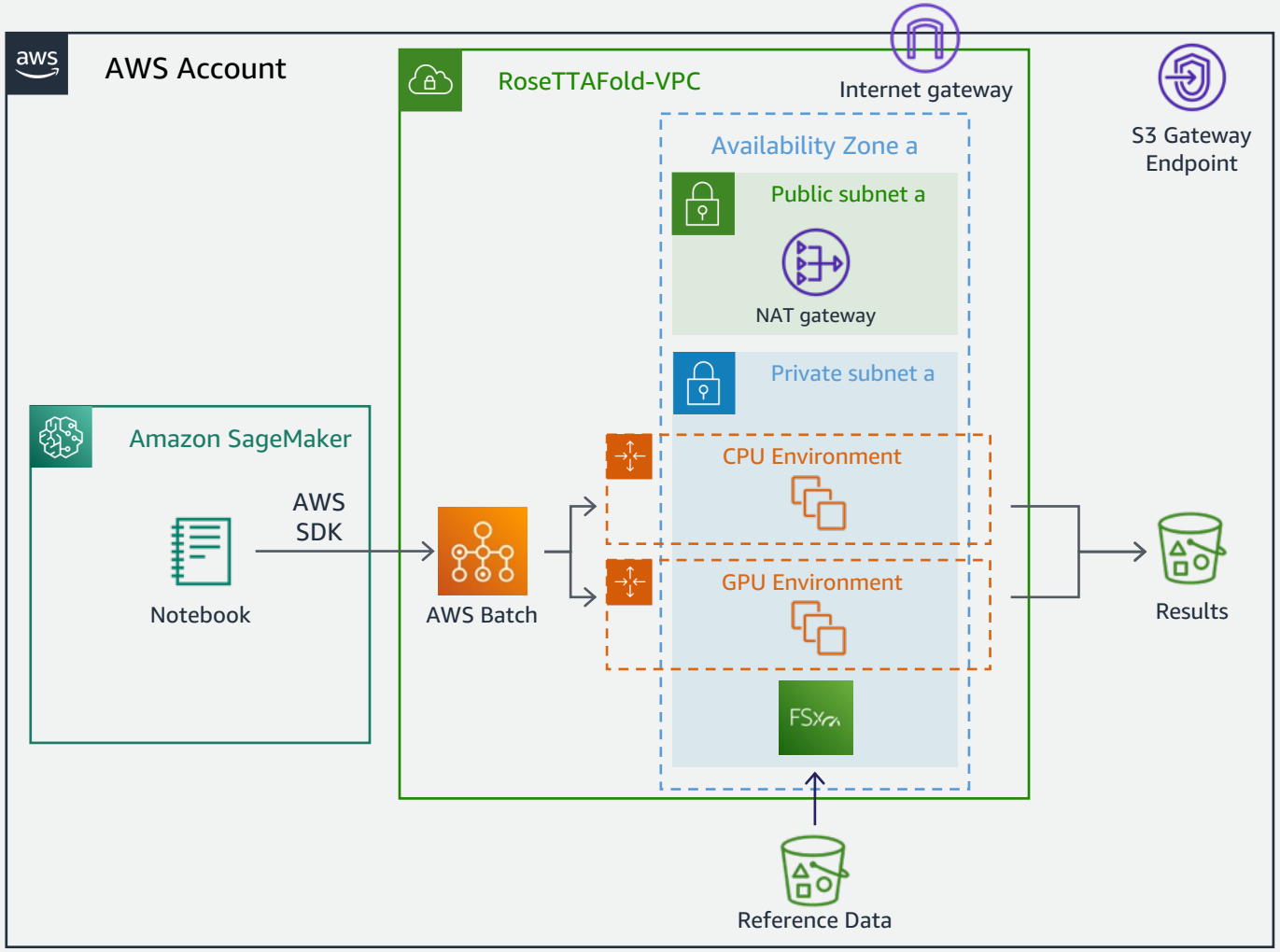
AWS-RoseTTAFold Architecture Overview



AWS-RoseTTAFold Deployment



AWS-RoseTTAFold Network Architecture



Cost Analysis

Fixed Costs

Service	Monthly Cost (USD)
NAT Gateways (1)	$40
FSx Lustre file system (SSD, 100 MBps/TB, 1.2 TB)	$228
Amazon S3 (50 GB)	$2
Total	**$270**

Typical Per-Job Costs

Service	Cost per Job (USD)
EC2 – CPU (1 hour on m4.4xlarge Spot with 5% interruption)	$0.38
EC2 – GPU (1 hour on g4dn.12xlarge Spot with 5% interruption)	$1.72
Total	**$2.10**

Benefits of Well-Architected Design

Operational Excellence

- Account owners can rapidly deploy infrastructure and containers using self-service CloudFormation and CodePipeline jobs.

Security

- All compute instances live within private VPC subnets and all data is encrypted at rest and in-transit.

Reliability

- AWS Batch jobs automatically restart on failure and scale horizontally across multiple AZs to meet demand.

Performance Efficiency

- Scientists can define custom vCPU, memory, and GPU requirements within Jupyter and use powerful instance types.

Cost Optimization

- Batch autoscaling policies minimize the total cost of ownership by scaling down instances when no longer needed.

Starting your ML journey

Training

Proof of concept

Production

Thank you!