
AWS
re:Invent
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LFS301

Emerging super compute strategies for life sciences R&D

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Agenda

Introduction to AWS for Health

Challenges and trends in biopharma research and discovery

Exploring the data and cloud continuum

Designing for scale

Developing a data-centric architecture

Whiteboarding and Q&A

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Accelerating scientific insights and time to patient care

Is my why

Steve Litster Ph.D
Senior Manager WWSO Compute Specialists, HCLS
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Using technology to save and improve lives

Is my why

Chris Chalfant (he/him)
BDSI HCLS Solution Architect
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AWS Health



Omics



Healthcare



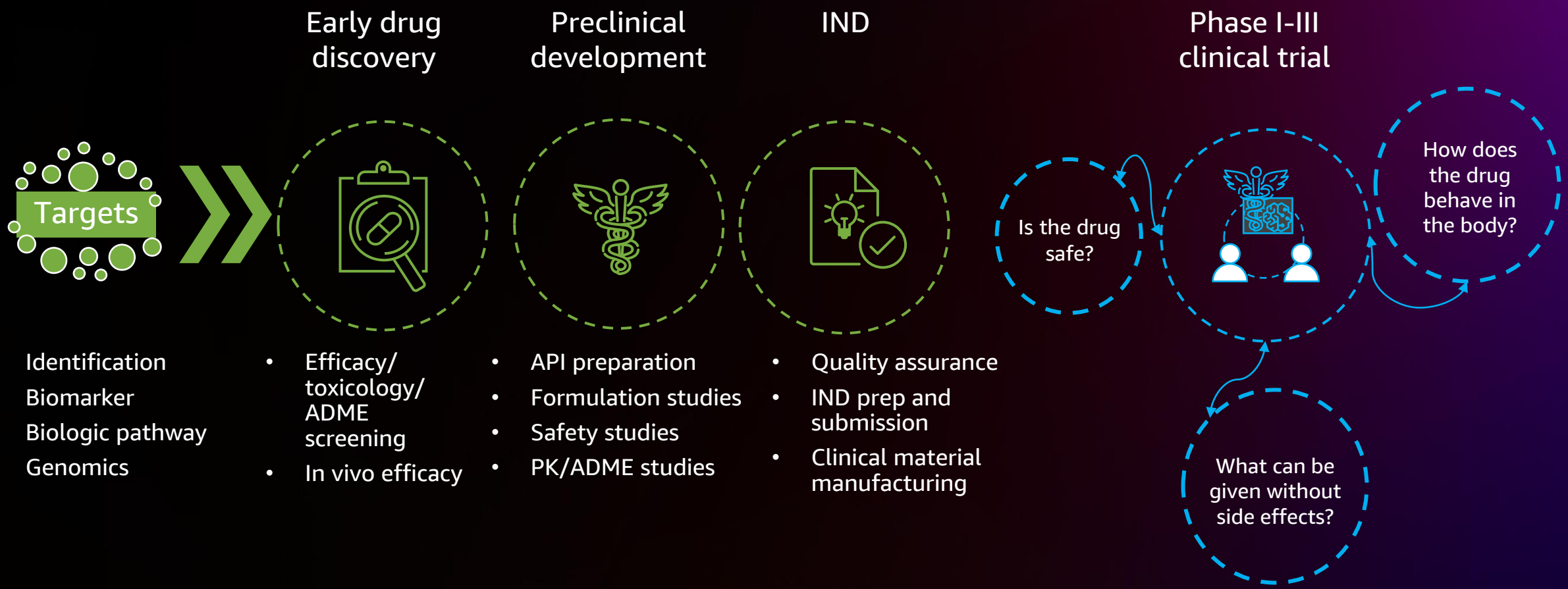
Life sciences

Accelerating innovations from benchtop to bedside

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Simple R&D drug discovery pipeline

ACCELERATING RESEARCH AND DEVELOPMENT



- Identification
- Biomarker
- Biologic pathway
- Genomics

- Efficacy/ toxicology/ ADME screening
- In vivo efficacy

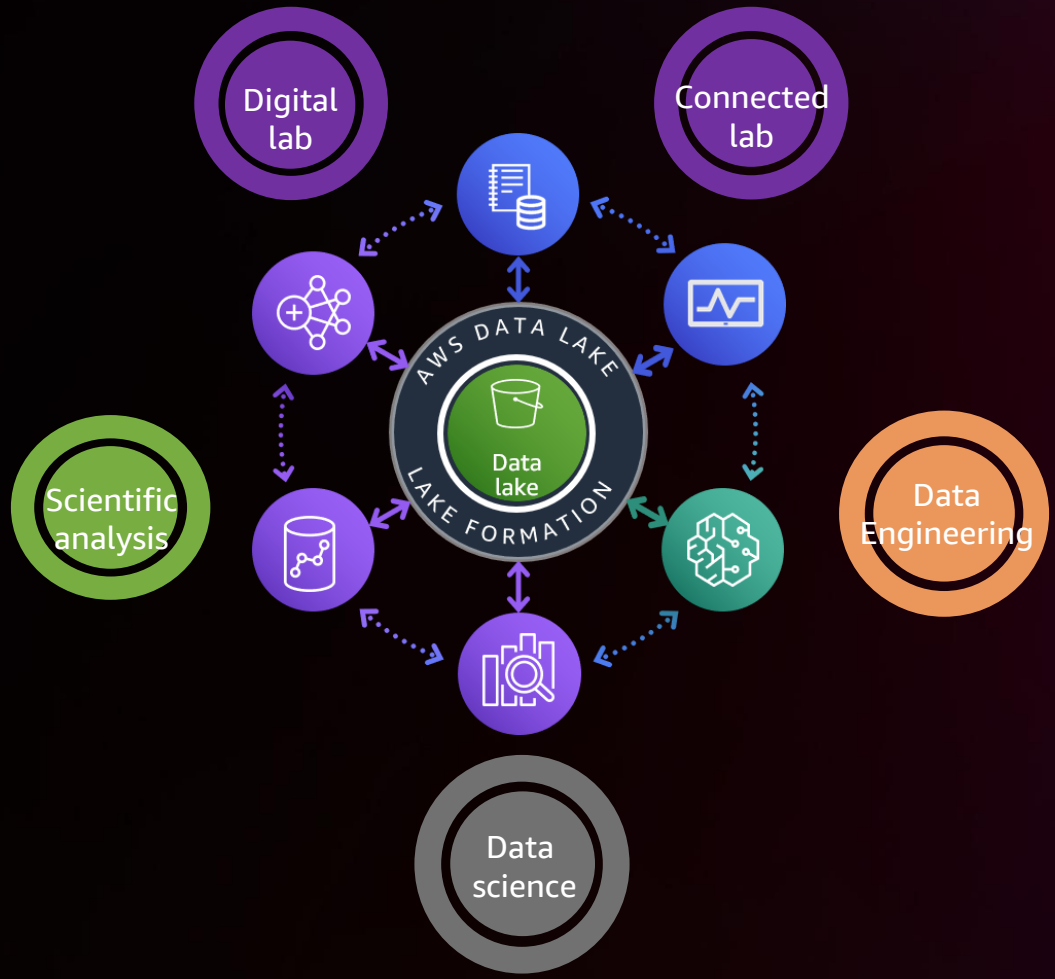
- API preparation
- Formulation studies
- Safety studies
- PK/ADME studies

- Quality assurance
- IND prep and submission
- Clinical material manufacturing

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Data continuum/data centric



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Data continuum/data centric

Applications for managing experiments, inventory, samples, robotics

Information systems engineer
Lab/automation engineer

Modeling, virtual screening, bioinformatics

Computational chemist
Bioinformatician
Data scientist

Machine learning (ML) and knowledge graphs, Elasticsearch

Data scientist
ML engineer



Instrument control and data harmonization

Wet-lab scientist
Lab systems engineer
Information systems engineer

Data cataloging, governance, and collaboration

Data analyst
Data engineer
Data architect

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Cloud continuum

AWS DELIVERING CLOUD WHERE CUSTOMERS NEED IT

AWS Regions



Compute & networking

Amazon EC2

Elastic Fabric Adapter (EFA)

Management

AWS ParallelCluster

NICE EnginFrame

Storage

Amazon FSx for Lustre

Amazon S3

Batch processing

AWS Batch

Visualization

NICE DCV

For most use cases

On premises

AWS Outposts

Metro centers

AWS Local Zones

5G networks

AWS Wavelength

AWS IoT Greengrass and FreeRTOS

AWS Snow Family

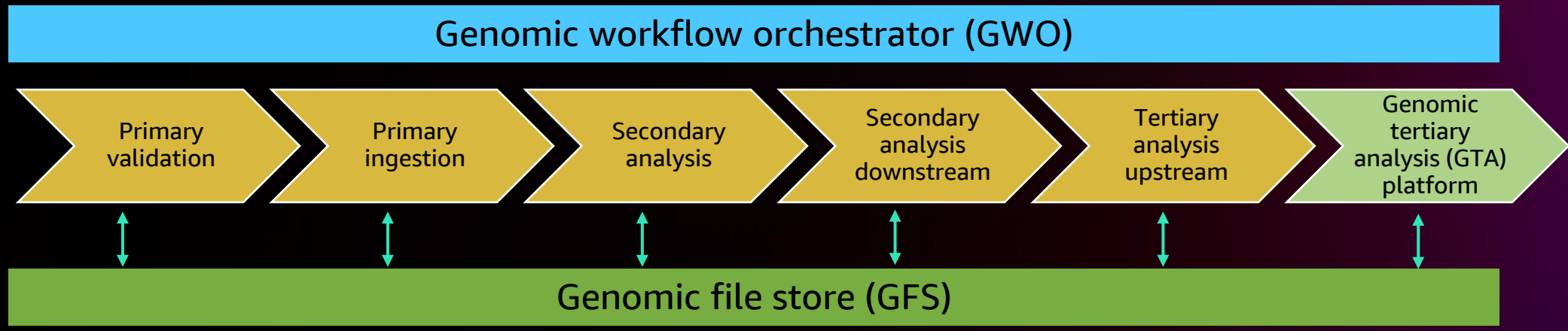
For low-latency, local data processing, data residency

Cloud continuum

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Design for scale

GENOMIC FILE STORE



Genomic file store (GFS)

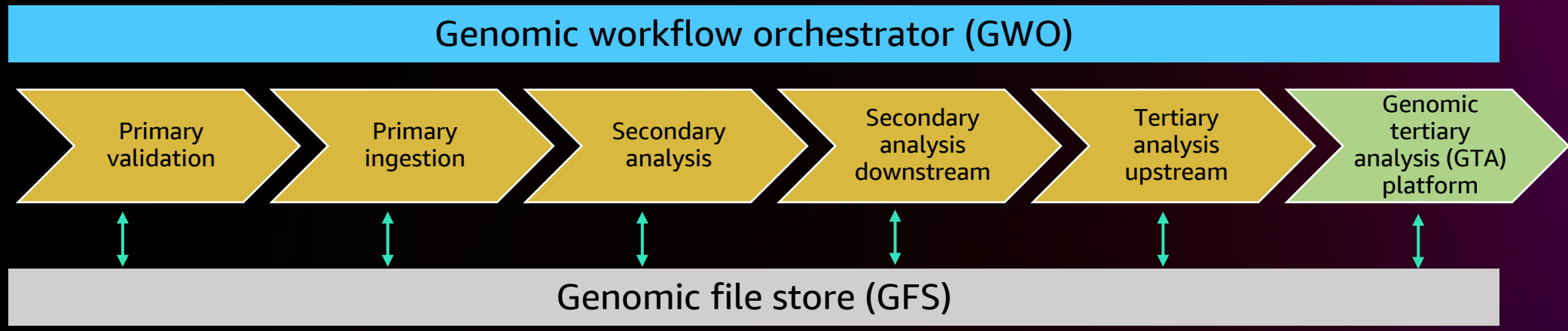
- **Amazon S3 object store**
  - Inventory and versioning
  - Encrypted using customer managed keys
  - Lifecycle management based on object level tags, per file type (bam, fastq)
  - Cost tracking per bucket
- **Busines defined metadata**
  - Associated with files at ingestion
  - Metadata validation rules
  - Producer, capture-kit, sequence type, sequence machine

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Design for throughput

GENOMIC WORKFLOW ORCHESTRATION



Genomic workflow orchestrator (GWO)

- Loosely coupled pipelines
- AWS Step Functions with parallel tasks
- AWS Lambda for coordination tasks
- AWS Batch for processing tasks
- Initiated on demand or automatically
- Track duration for all tasks
- Track who, what, when

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AWS HPC life science stack

BUILDING FIT FOR PURPOSE ARCHITECTURES

Orchestration/automation



Visualization



Scientific applications

Genomics

NextFlow, RNA-Seq, WGS, Cromwell

Imaging

Relion, CryoSparc, CellProfiler

Modeling and simulation

CFD,NONMEM, Ansys, R

Computational chemistry

CryoSparc, OpenEye Schrodinger,

Informatics data science

R, SAS, TensorFlow, Jupyter Notebooks

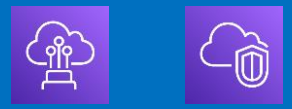
Compute



Storage



Networking



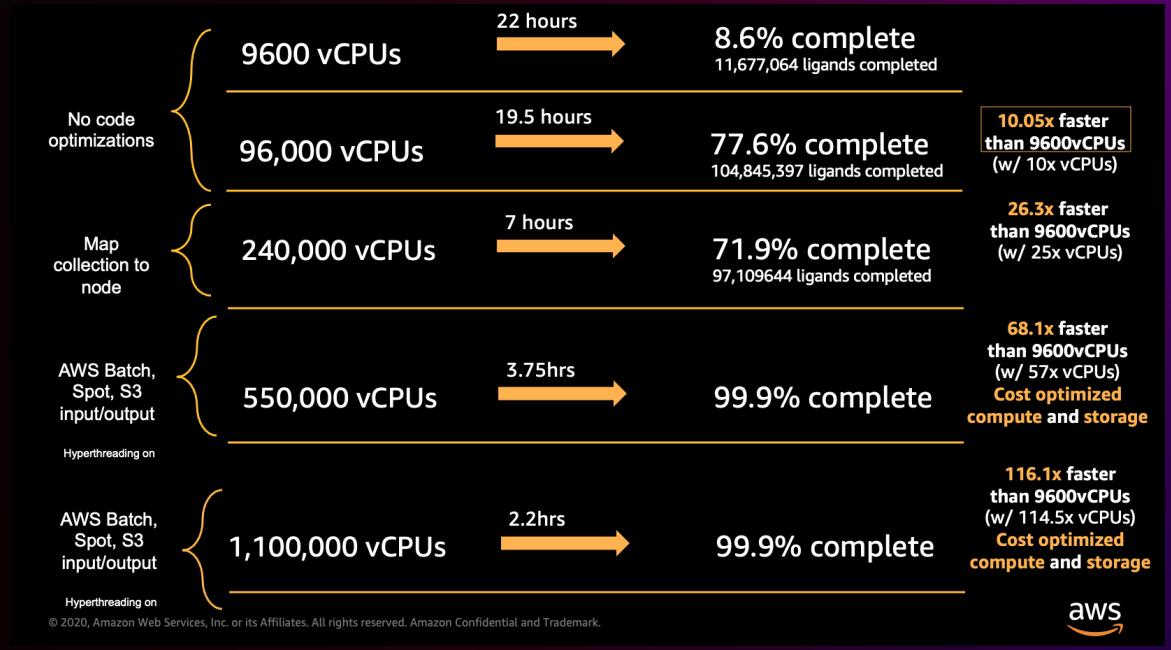
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VirtualFlow

OPEN SOURCE VIRTUAL SCREENING PLATFORM DEVELOPED BY HARVARD MEDICAL SCHOOL

- 2 modules
  - VirtualFlow ligand preparation (VFLP)
  - VirtualFlow virtual screening (VFVS)
    - Optional re-screening step to increase accuracy for selected molecules
- ZINC15 (>450 M molecules) and REAL (>1.4 B molecules) compound libraries available
- Provides a narrowed down list of small molecules for lab experimental analysis



Scaled to 2.5 M vCPUs

AWS Batch

Source: https://www.nature.com/articles/s41586-020-2117-z and https://virtual-flow.org/

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AWS + Children's National Hospital

Customer obsession = Patient obsession

Collect pins at the AWS for Health Lounge from child artists who are also patients at Children's National Hospital – learn about their inspiration and their **why**





Artwork provided by Zahara, age 13, patient with sickle cell

"I drew a cherry blossom because I love going to the DC Cherry Blossom Festival in the spring. The care I get at Children's National allows me to do all the things I love and have lots of fun!"

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AWS Health Lounge

Connect with **AWS Health experts** and other attendees in our dedicated lounge space for **informal discussions and networking**

Explore **AWS healthcare & life sciences demos** and new additions to the AWS for Health portfolio

Location: AWS Industries Networking Lounges; Caesars Forum Main Hall



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Thank you!



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