

HPC on AWS: Shaping the Future of Virtual Humans Together

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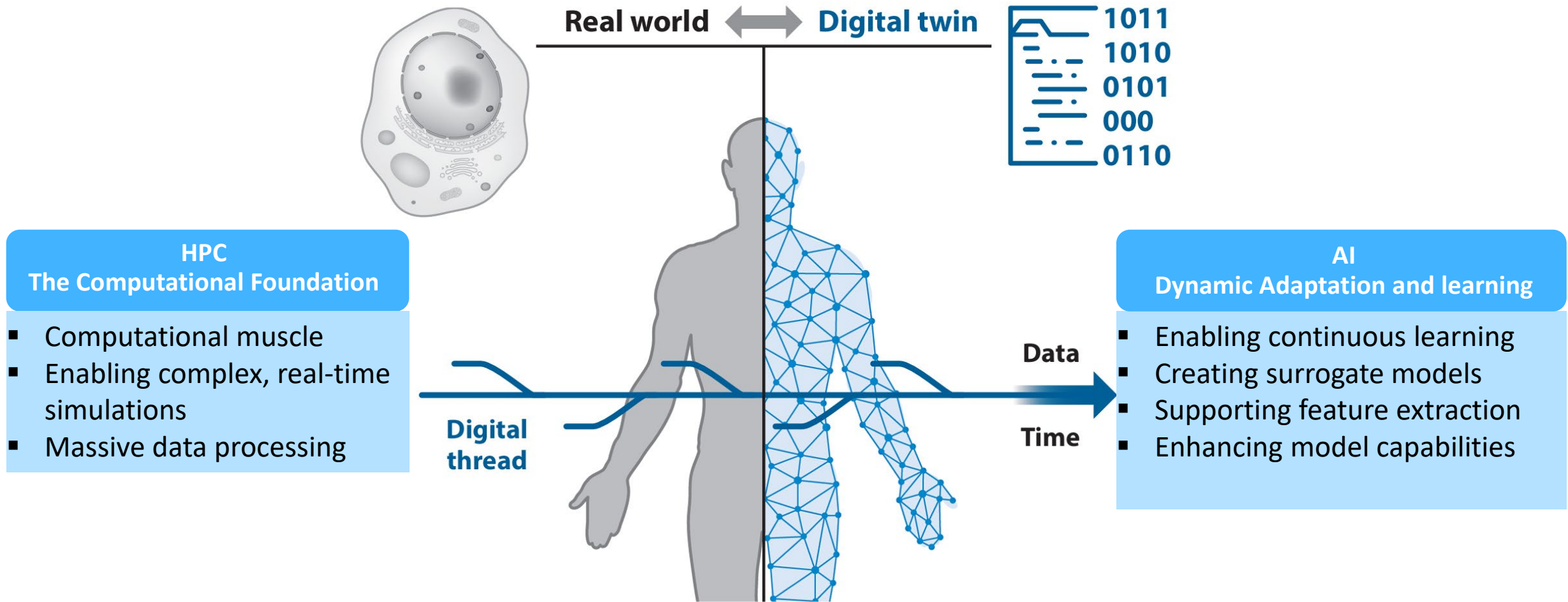
HPC Specialists, AWS



Agenda

- Virtual Human Twins in Drug Development
- The Technology Behind the Innovation
- Accelerating your Breakthroughs Together

The Critical Role of HPC and AI in Virtual Human Twins

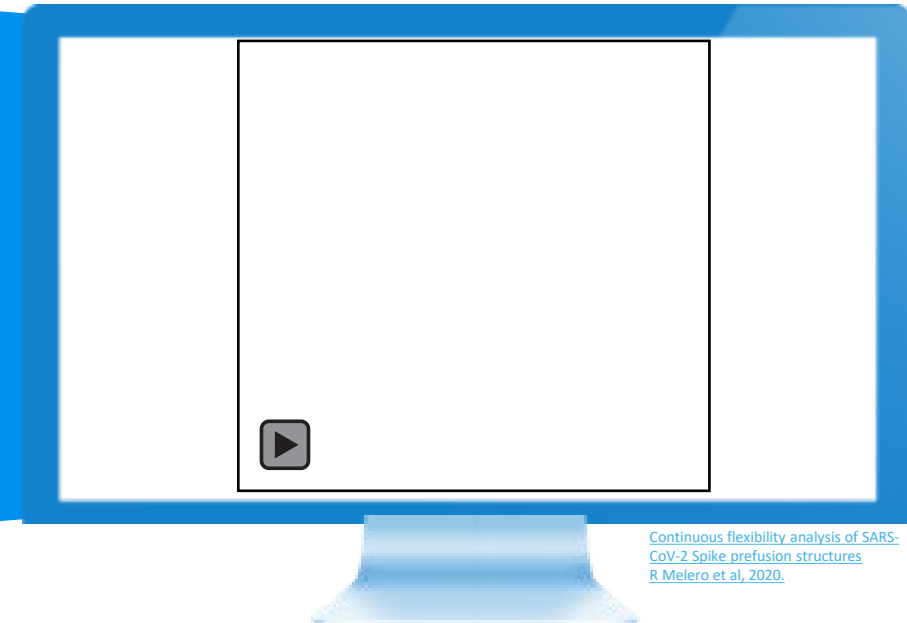


Accelerating Drug Development

\$6B *R&D per drug* | **12-15 years** *per drug* | **<10% success rate**



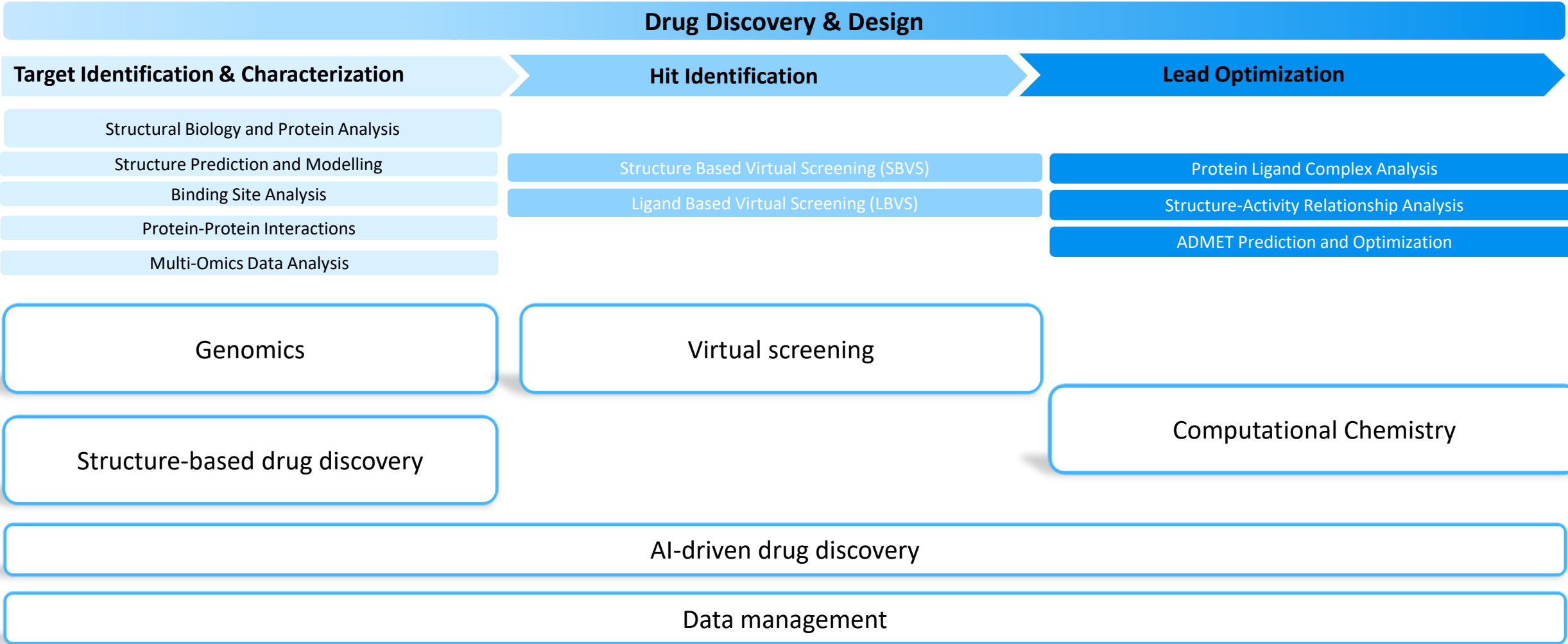
From bench to
in silico



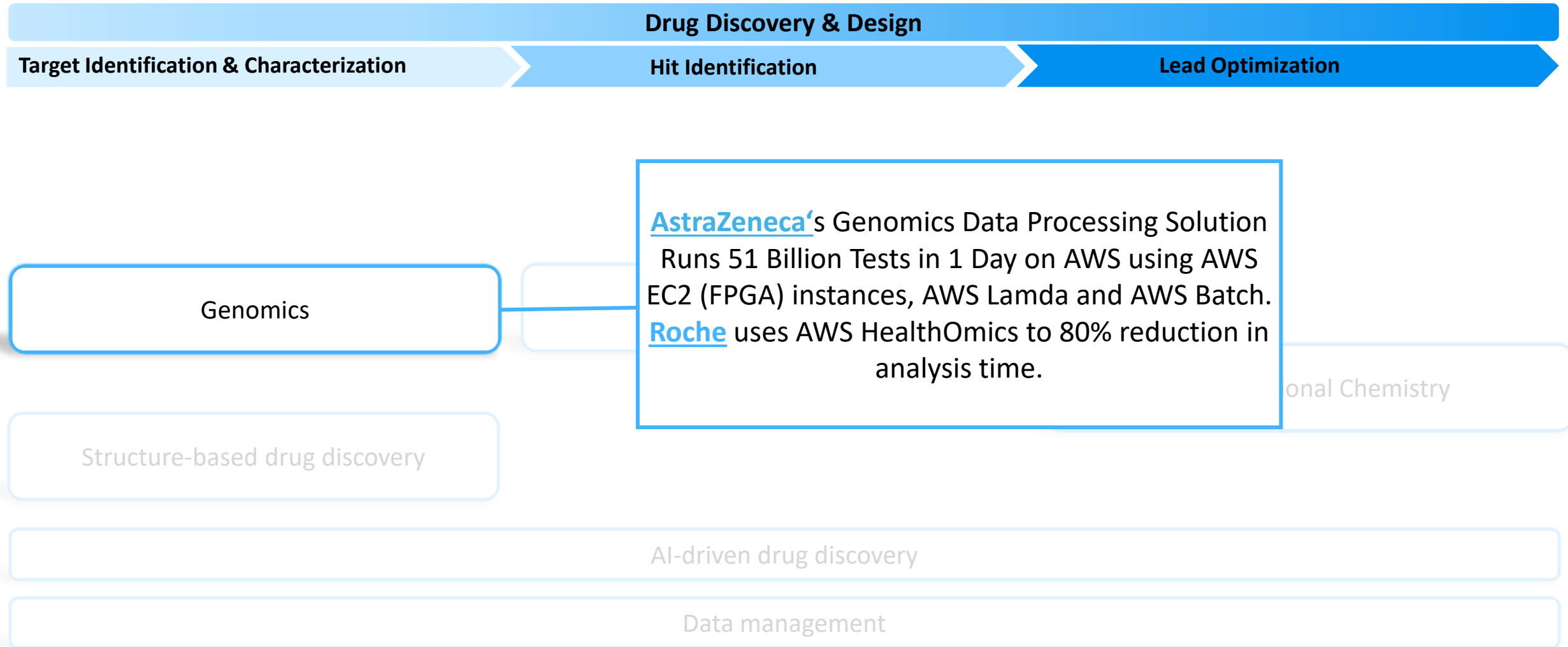
[Continuous flexibility analysis of SARS-CoV-2 Spike prefusion structures](#)
R. Melero et al, 2020.



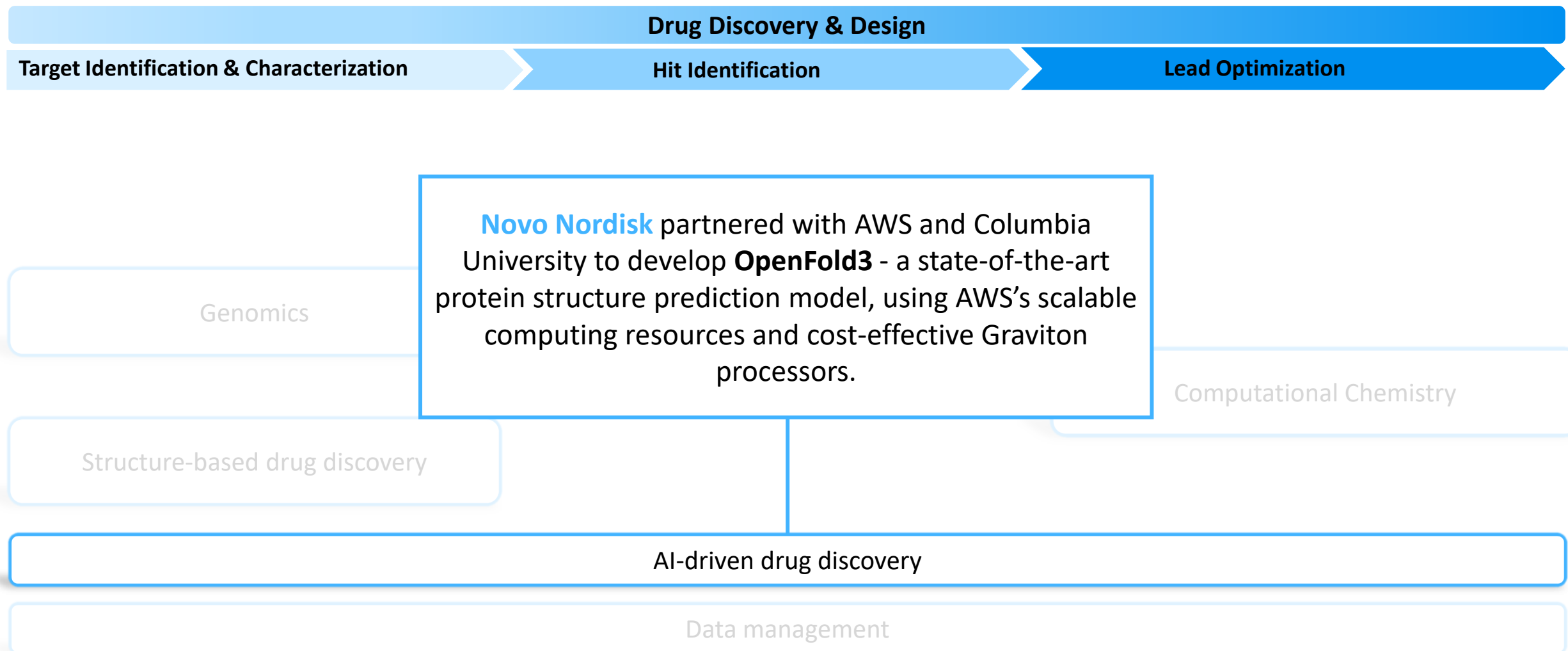
Established Capabilities in R&D



Removing Bottlenecks in Genomics Processing and Analysis



Accelerating Protein Structure Prediction with OpenFold3



Enabling Digital Twins: A Multi-Layered Approach

USE CASES

Reduce from 90 to 30 days the time to characterize a new target protein using cryo-EM

Identify and characterize potential binding pockets, evaluating their druggability and validating predictions

Crystal structure prediction (CSP) to determine the most developable isophorm

Screening a library of 10,000+ compounds (small molecules) against a new target

Predict the structure of 500+ protein sequences

WORKFLOWS

Structure Based Virtual Screening

Cryo-EM

Molecular Dynamics

CHALLENGES

Scale complexity

Real-time processing

Combining heterogeneous multi-omics data

TECHNOLOGY ENABLERS

High Performance Computing

Artificial Intelligence

AWS Digital Twin Framework

DATA FOUNDATIONS

PARTNERS



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HPC, the Computational Muscle

TECHNOLOGY ENABLERS

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Artificial Intelligence

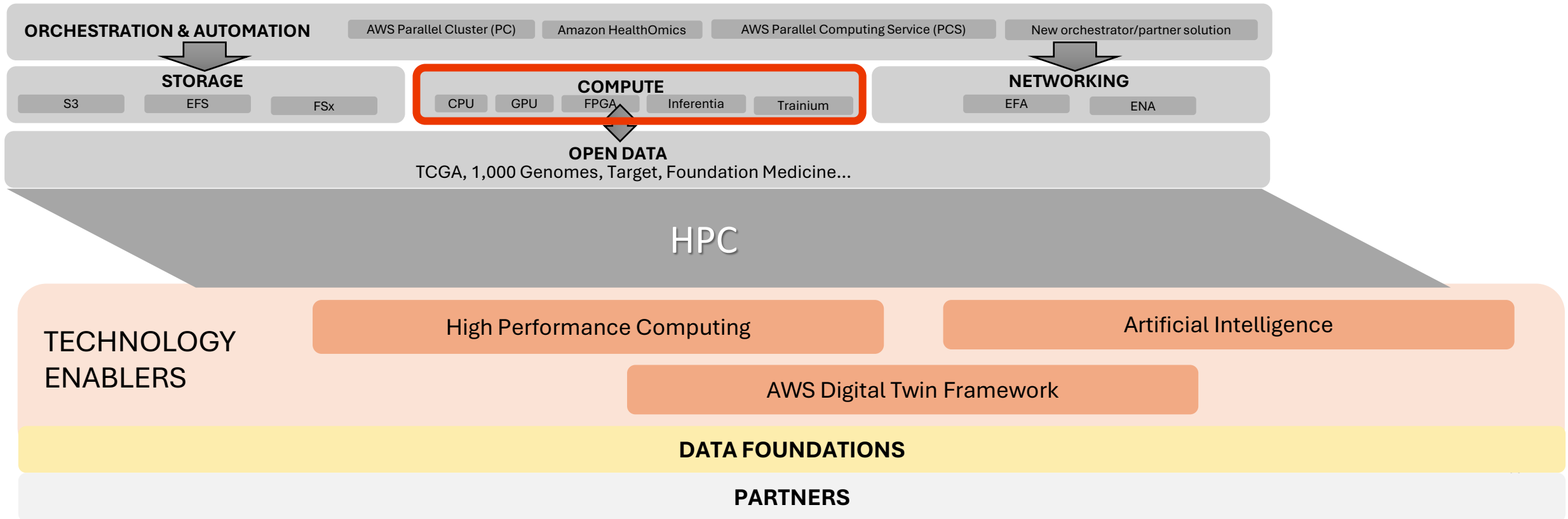
AWS Digital Twin Framework

DATA FOUNDATIONS

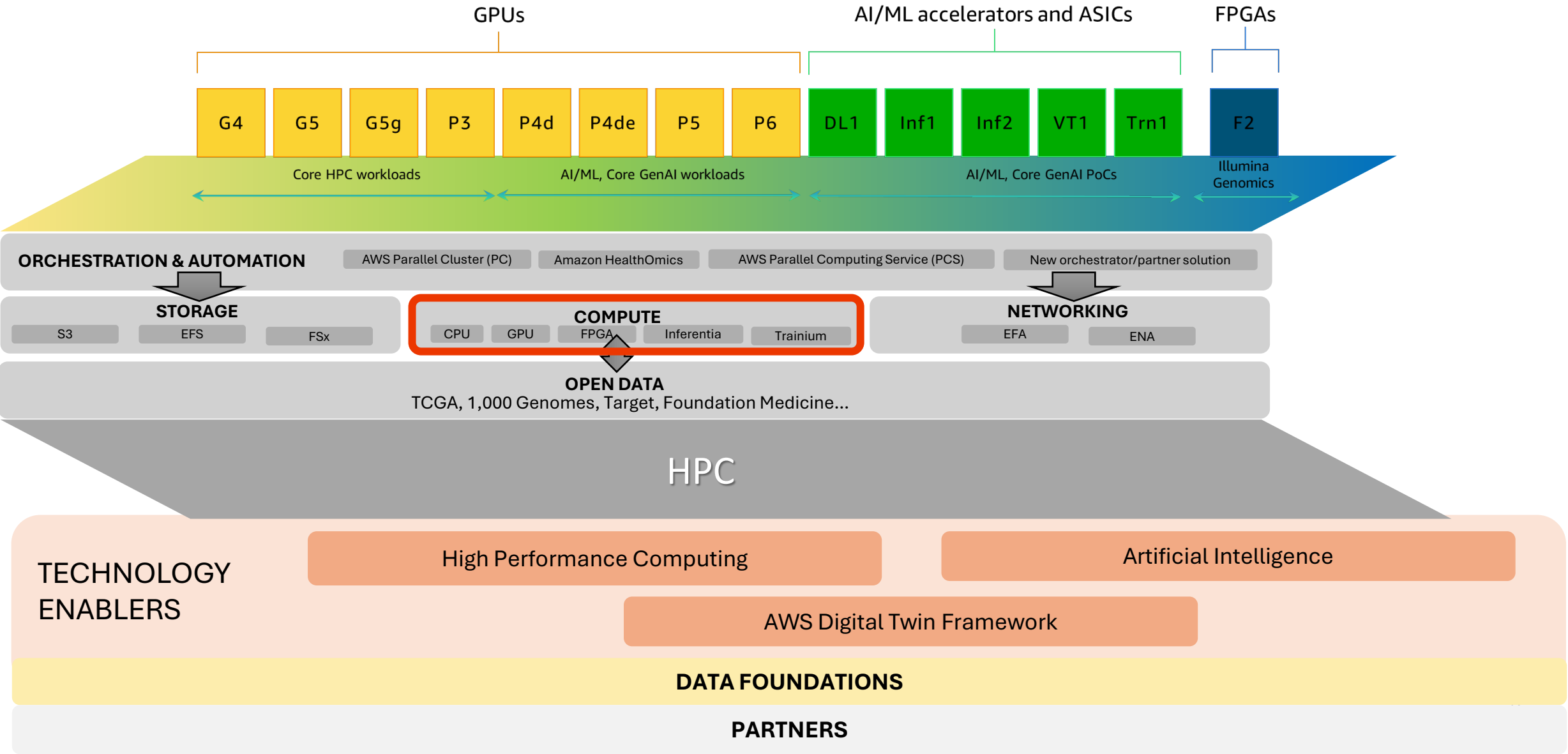
PARTNERS



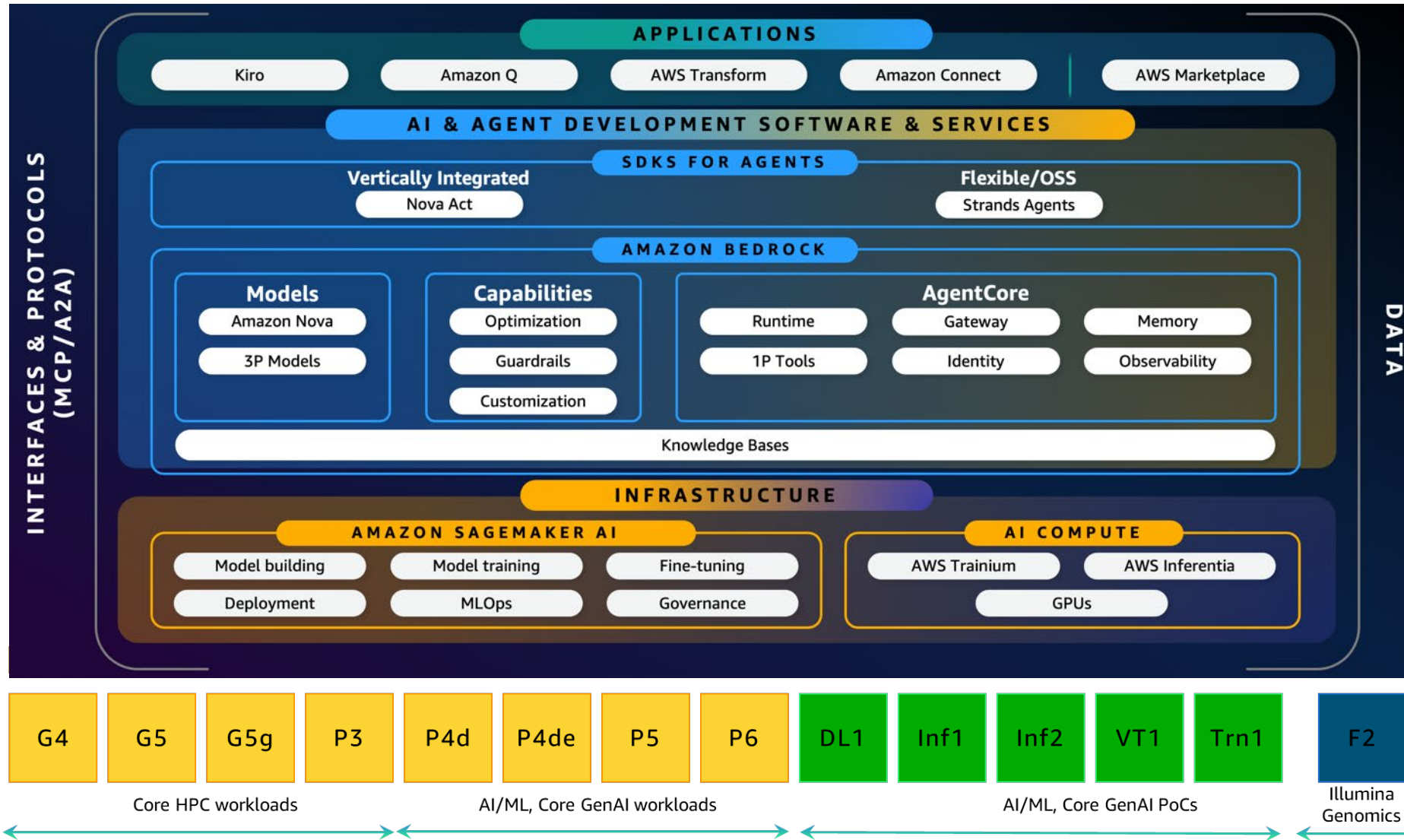
HPC, the Computational Muscle



The Right Technology for the Right Use Case at the Right Time

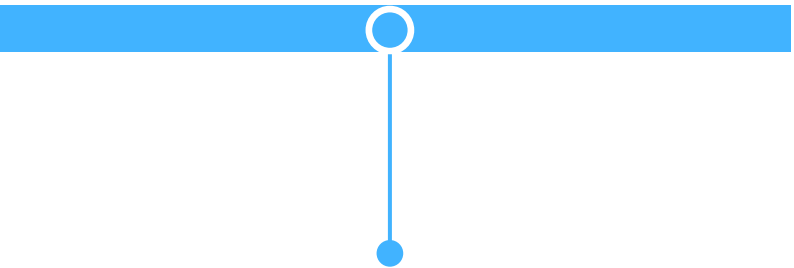


AI, the Computational Brain



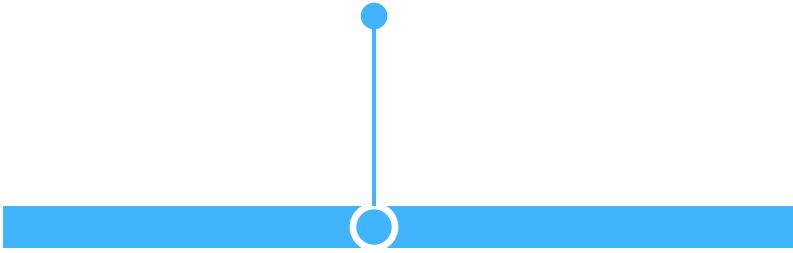
This is How We Engage

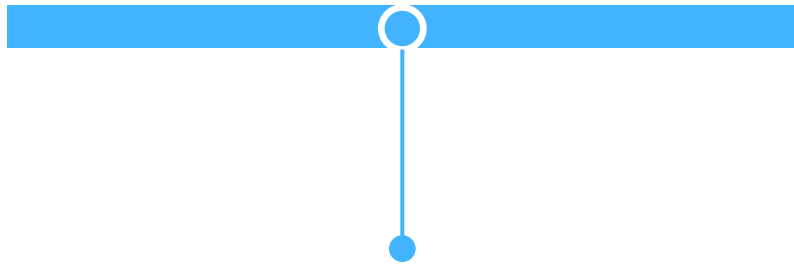
- Collaborate as scientific peers
- Define outcomes together
- Understand your workflows
- Shape our roadmap



**Scientific Expertise &
Outcome-based
approach**

**Hands-on Technical
Exploration**

- 
- Evaluate cutting-edge architectures
 - Benchmark across environments
 - Optimize workflows
 - Integrate new tools
 - Design advanced infrastructure
 - Co-develop tailored features



**Your Extended
Scientific Team**

- Work as team extensions
- Drive computational innovation
- Explore and validate approaches
- Connect with partners
- Support knowledge sharing
- Facilitate technical events
- Shape future technologies

Your Partner for Virtual Human Twin



AWS SPECIALIST AND PARTNER ORGANISATION

HEALTHCARE AND LIFE SCIENCES

TECHNOLOGY
DOMAINS &
PARTNERSHIPS

Please reach out to collaborate!

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