Composable Infrastructure for Technical Computing

IBM Spectrum Scale US User Group Meeting 2018 Cambridge, MA

May 17, 2018

Ulf Troppens Client Engagements & Solutions Delivery IBM Spectrum Scale Development

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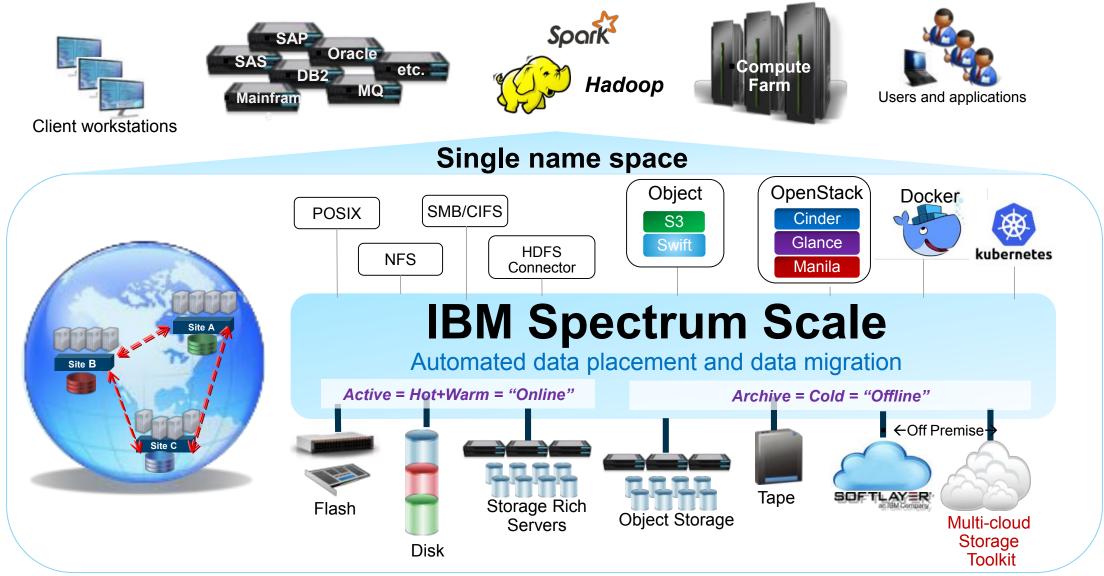
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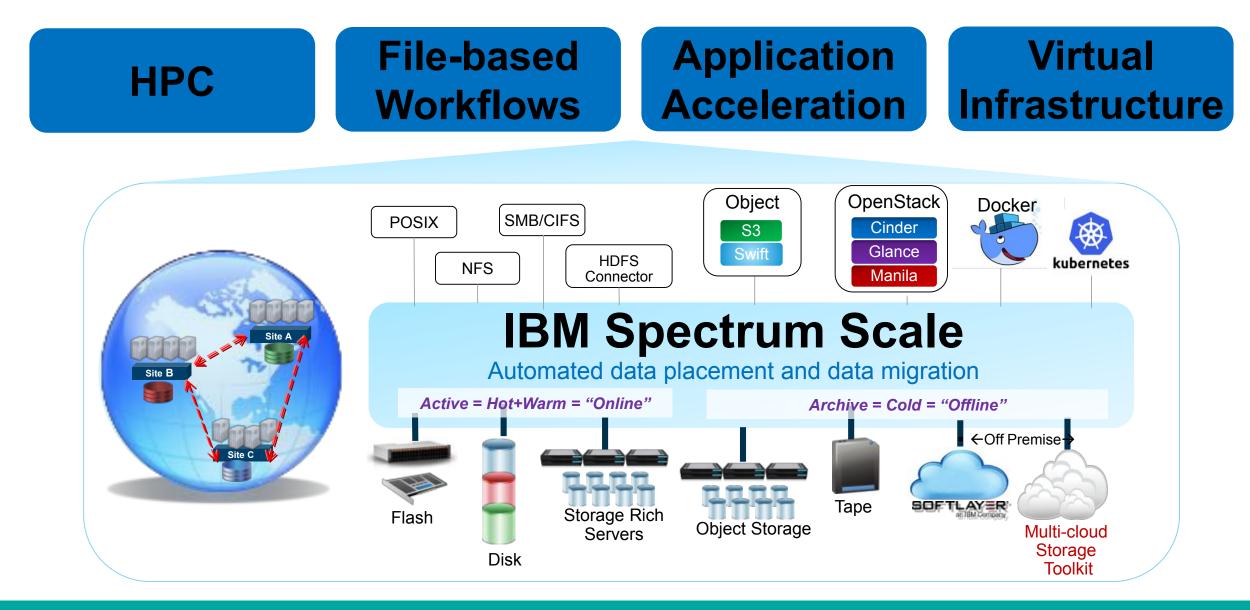
Outline

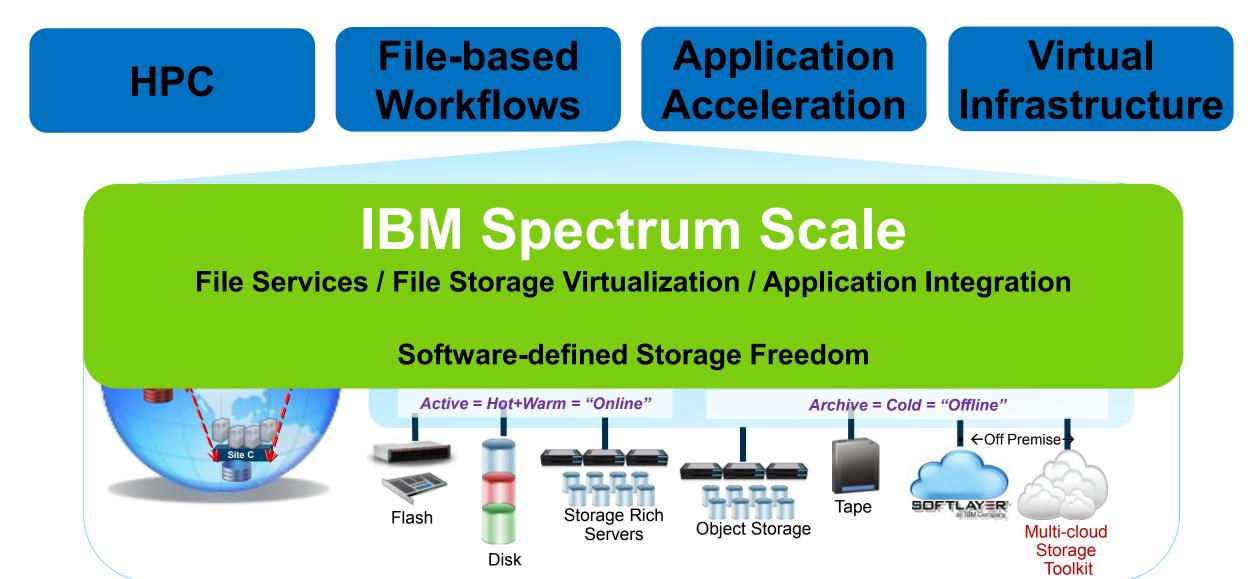
Motivation

Composable Infrastructure for Genomics Medicine Workloads

Unleash New Storage Economics on a Global Scale









IBM Spectrum Scale

File Services / File Storage Virtualization / Application Integration

Software-defined Storage Freedom

Freedom of Choice

Choose Storage which Meets your Needs Flash // Disk // Tape // Object // Cloud



IBM Spectrum Scale

File Services / File Storage Virtualization / Application Integration

Network Software-defined Storage Freedom

Freedom of Choice

Choose Storage which Meets your Needs Flash // Disk // Tape // Object // Cloud

Engagement Process

(4)

(3)



IBM Spectrum Scale

File Services / Filesystem Virtualization / Application Integration

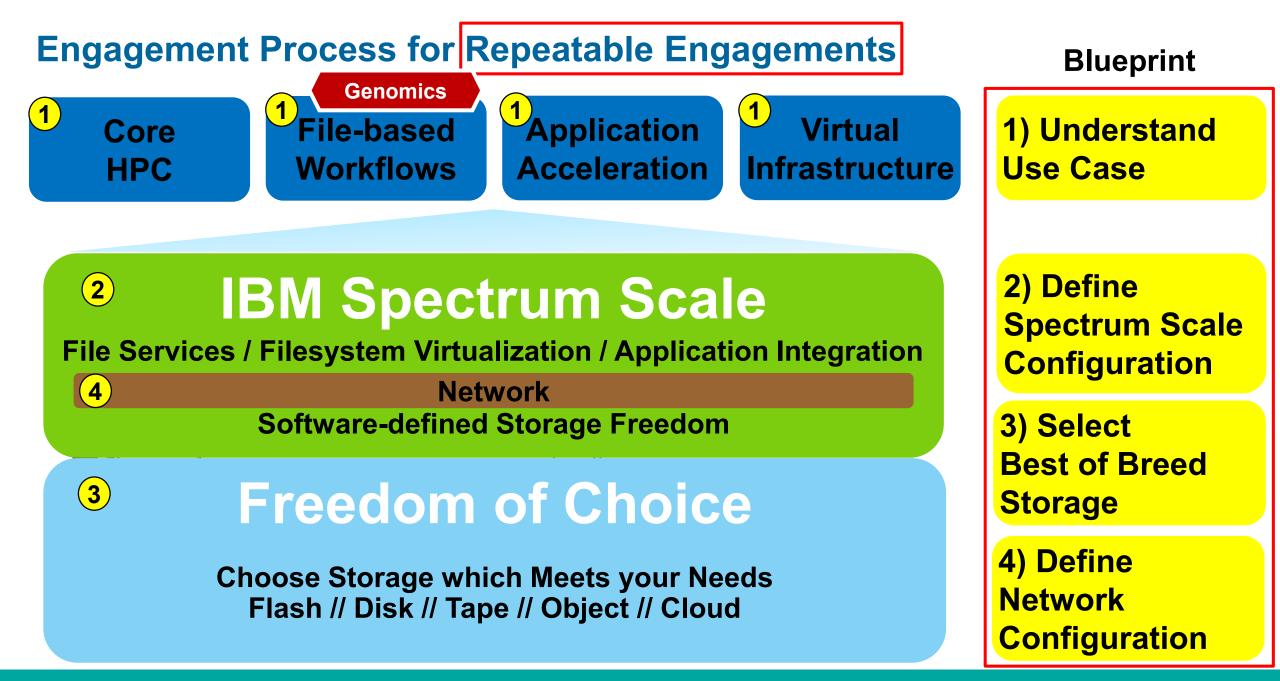
Network Software-defined Storage Freedom

Freedom of Choice

Choose Storage which Meets your Needs Flash // Disk // Tape // Object // Cloud 2) Define Spectrum Scale Configuration

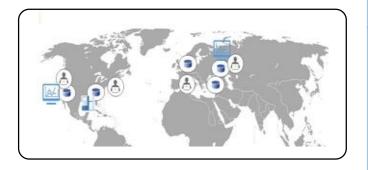
3) Select Best of Breed Storage

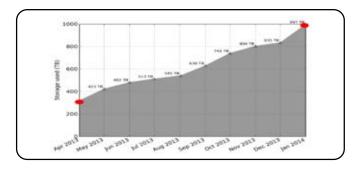
4) Define Network Configuration



Genomics

IBM Storage & SDI

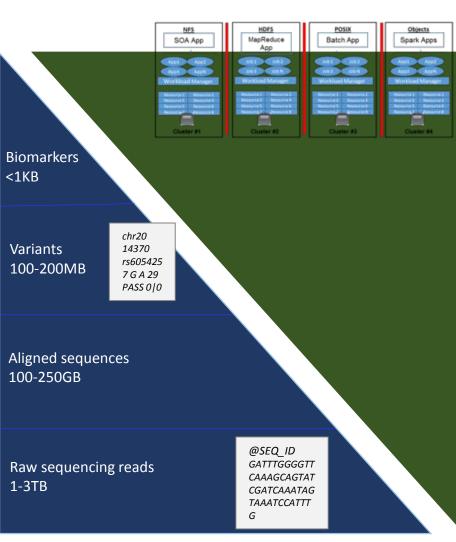


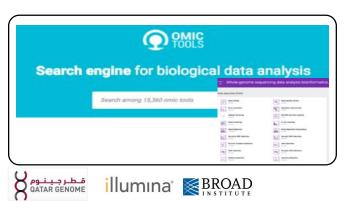


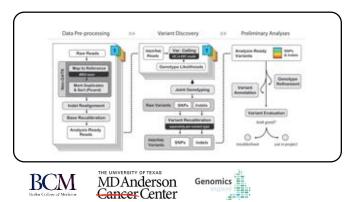


MDAnderson Cancer Center

Mount Sinai





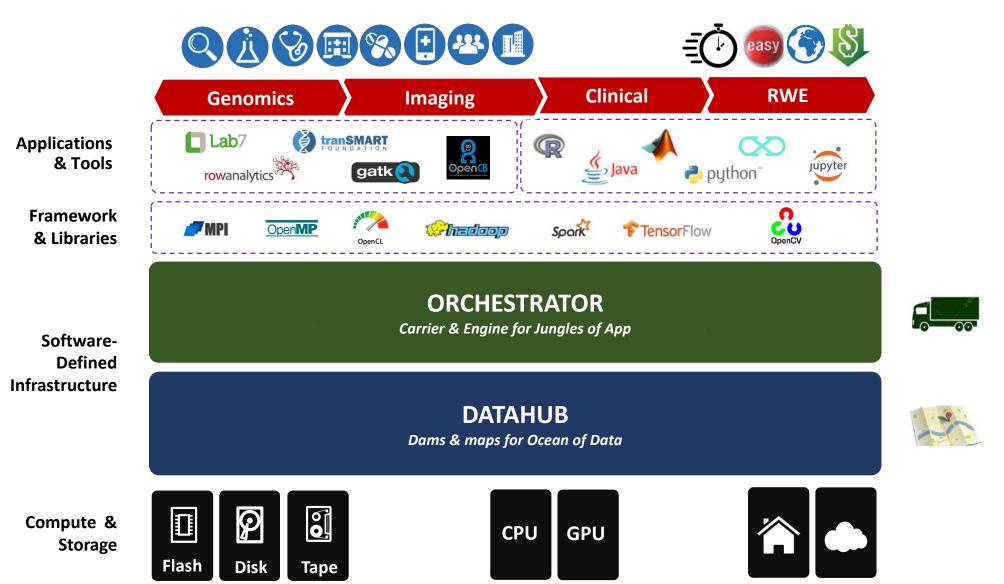


Ion Proton

Ion PGM

Illumina MiSeq Roche-454 GS-FLX

High Performance Data & AI (HPDA) Architecture



http://www.redbooks.ibm.com/abstracts/redp5210.html?Open

IBM Storage & SDI

Success Stories

Reduced time to completion for long running jobs while increasing resource utilization

"Analyzing hundreds of samples in parallel on a regular basis requires a robust HPC system to handle the load properly. From our experience, IBM systems has proven to be reliable in helping us address this technical requirement."

Dr. Mohamed-Ramzi Temanni, Manager, Bioinformatics Technical Group at Sidra Medical and Research Center



More than 3x performance using 1/3 the nodes

"Delta will enable quantitative analysis and interpretation of large biological genomics data generated at LSU".

Gus Kousoulas, associate vice president for research and economic development, Louisiana State University 96% reduction in the runtime of a standard genome analysis pipeline

"With IBM Cloud, and in particular its highperformance compute infrastructure and services, we found the ideal platform for building a comprehensive cloud solution for genomics".

Christopher Mueller, Ph.D., President and Chief Technology Officer of Lab7 Systems



Accelerating genetics research and medicine 500% with IBM SDI

As a result of replacing its open-source workload manager—which crashed on a monthly basis with IBM Spectrum LSF to improve both reliability and scalability, the team has seen core dumps fall to zero over a one-year period while overall scalability increased to 500,000 jobs per queue.

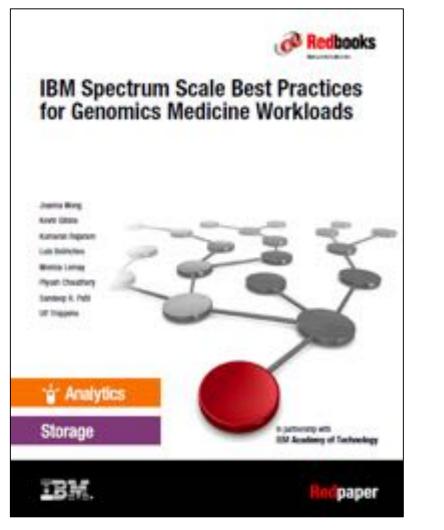
Icahn School of Medicine, Mount Sinai



Outline

- Motivation
- Composable Infrastructure for Genomics Medicine Workloads

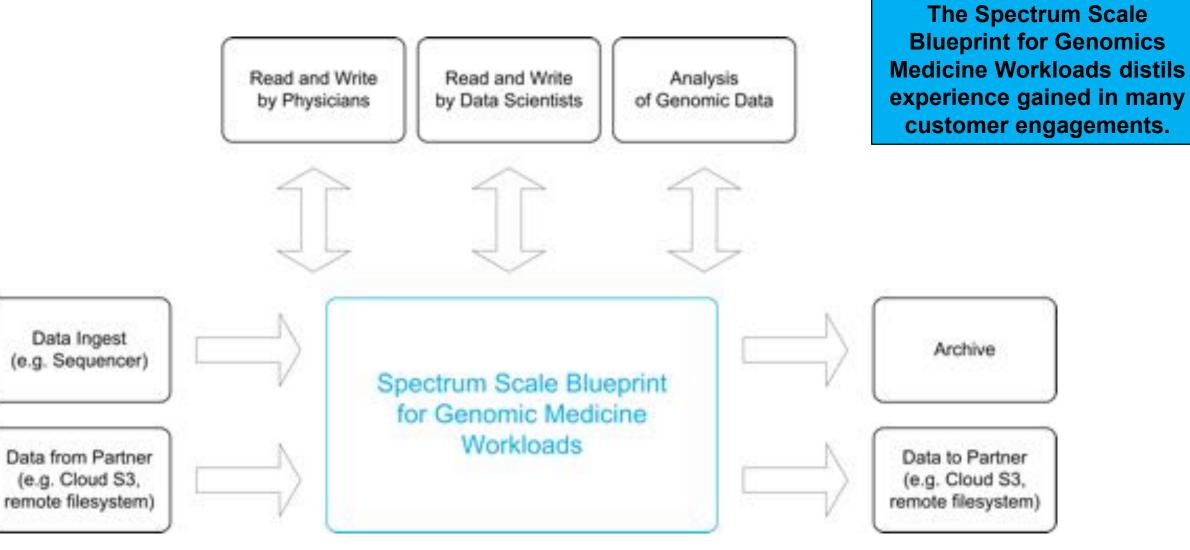
Summary



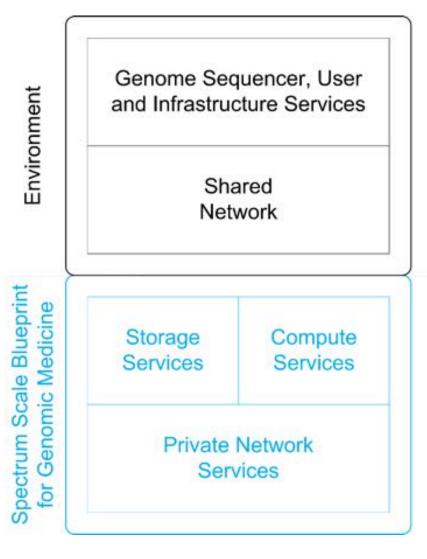
- IBM is helping life science companies across the globe to accelerate research and drug development by providing infrastructure to store, share and manage huge amounts of genomics data and to analyze it quickly.
- IBM distilled the experience gained in the many customer engagements in the IBM Spectrum Scale Best Practices for Genomics Medicine Workloads.
- The best practices guide provides composable infrastructure based on expertly engineered building blocks that enable IT architects to customize deployments for varying functional and performance needs.
- The modular approach allows to integrate selected building blocks into the customer's already existing infrastructure to protect already made investments.

System Context

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Composable Building Blocks



Storage Services

Scale-able Storage Cluster to store, manage and access genomics data.

Compute Services

• Scale-able **Compute Cluster** to analyze genomics data.

Private Network Services

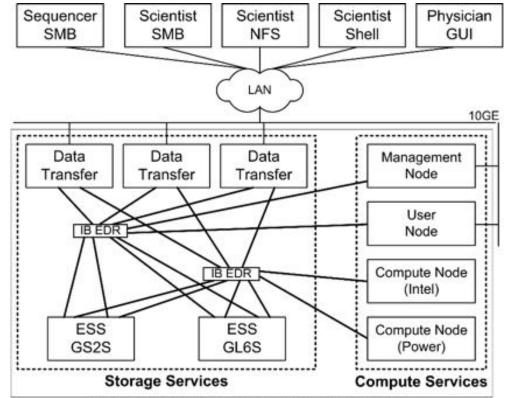
- High-speed Data Network, not connected to data center network.
- **Provisioning Network** and **Service Network** for administrative login and hardware services, optionally connected to shared campus network.

Shared Network

- User Login to submit and manage batch jobs and to access interactive applications.
- High-speed NFS and SMB Data Access, connected to shared campus network.
- WAN Optimization for fast and secure remote access to enable **collaboration across sites and institutions**.

Example questions for Genomics





Spectrum Scale Blueprint for Genomic Medicine

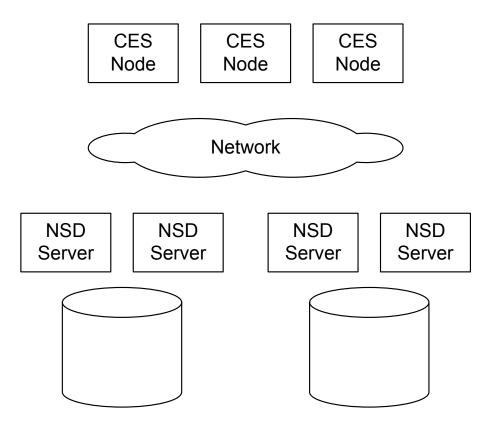
➔ Best Practices Guide includes one specific example environment.

Questions for Storage Services

- How many Genomes can be stored?
- How many Genomes can be processed per day?
- How many file systems to configure?
- What block size to configure for each file system?
- What other end-to-end tuning is required?
- Which node will be connected with how many InfiniBand links?
- Which nodes to configure as quorum node?
- What will change with Spectrum Scale 5.0?

Example questions for high-performance file services

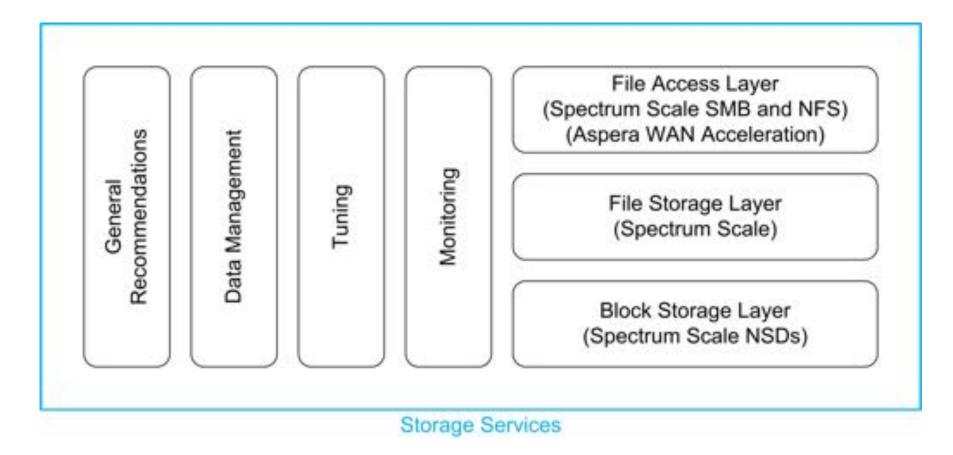




Questions for Storage Services

- How much data can be stored?
- How many MB/s can be read/written?
- How many operations can be served?
- What block size to configure for the file system?
- What other end-to-end tuning is required?
- What is the preferred network technology?
- What is the preferred network topology?
- Which nodes to configure as quorum node?
- What needs to be monitored and how?
- What will change with Spectrum Scale 5.0?

Storage Services - Composable Building Blocks

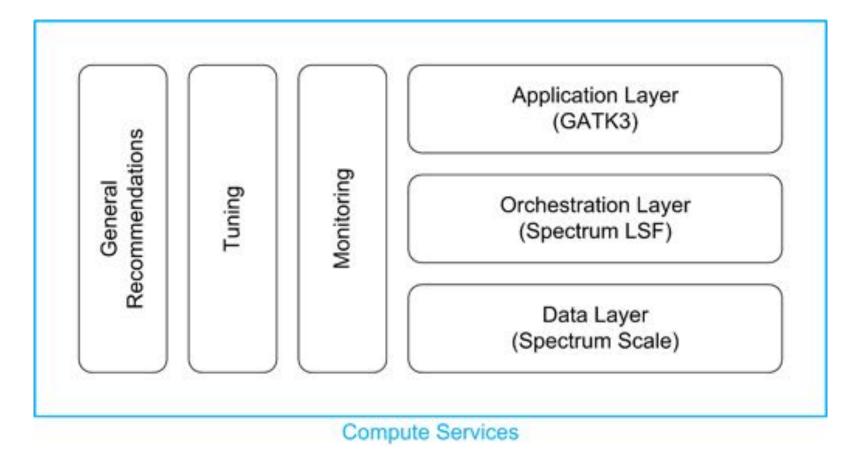


A set of expertly engineered building blocks enable IT architects to compose solutions that meet customers varying performance and functional needs.

Capabilities - Blueprint V1.1 - Storage Services

- To enable access to genomics data the Storage Cluster provides:
 - Data Transfer Nodes for secure high-speed external access via NFS and SMB to ingest data from genomic sequencers, microscope, etc., for access by data scientists/physicians
 - WAN Acceleration for collaboration across sites and institutions
 - Secure high-speed internal access for analysis on Compute Cluster
- To effectively store and manage genomics data the Storage Cluster provides:
 - Scale-out architecture that is capable to store data from a few 100 TB to Tens of PB of file data
 - End-to-end checksum to ensure the data integrity all the way from the application to the disks
 - **Quota Management** for user and project groups (future)
 - **Snapshots** for user and project groups (future)
 - Integrated Back-up and Fast Restore of PBs of data (future)
 - Data Management GUI to configure and monitor storage resources
 - Optional Professional Services ranging from management of daily operation to consultancy for major configuration changes
- → Blueprint capabilities have been reviewed with and prioritized by IBM Healthcare and Life Science team.
- ➔ Blueprint capabilities are written in a product neutral language to emphasize end user requirement.

Compute Services - Composable Building Blocks



A set of expertly engineered building blocks enable IT architects to compose solutions that meet customers varying performance and functional needs.

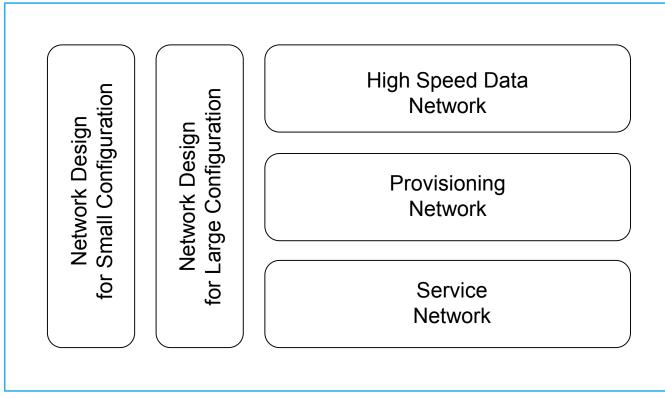
IBM Storage & SDI

Capabilities - Blueprint V1.1 - Compute Services

- To enable the **analysis of genomics data** the **Compute Cluster** provides:
 - User GUI for physician/data scientist to submit and manage batch jobs and to create and manage custom workflows
 - Workload Management GUI for IT administrator to view cluster status and utilization
 - Secure **high-speed access** to files stored on Storage Cluster
- Scaling
 - A **Workload Scheduler** enables high-throughput execution of batch jobs
- Performance
 - Tuning Recommendations supporting the "Broad Institute GATK Best Practices on IBM reference architecture"
- Node Types
 - **Power and/or x86-64 Nodes** for batch processing and for interactive login to access the resources

- → Blueprint capabilities have been reviewed with and prioritized by IBM Healthcare and Life Science team.
- → Blueprint capabilities are written in a product neutral language to emphasize end user requirement.

Network Services - Composable Building Blocks



Private Network Services

A set of expertly engineered building blocks enable IT architects to compose solutions that meet customers varying performance and functional needs.

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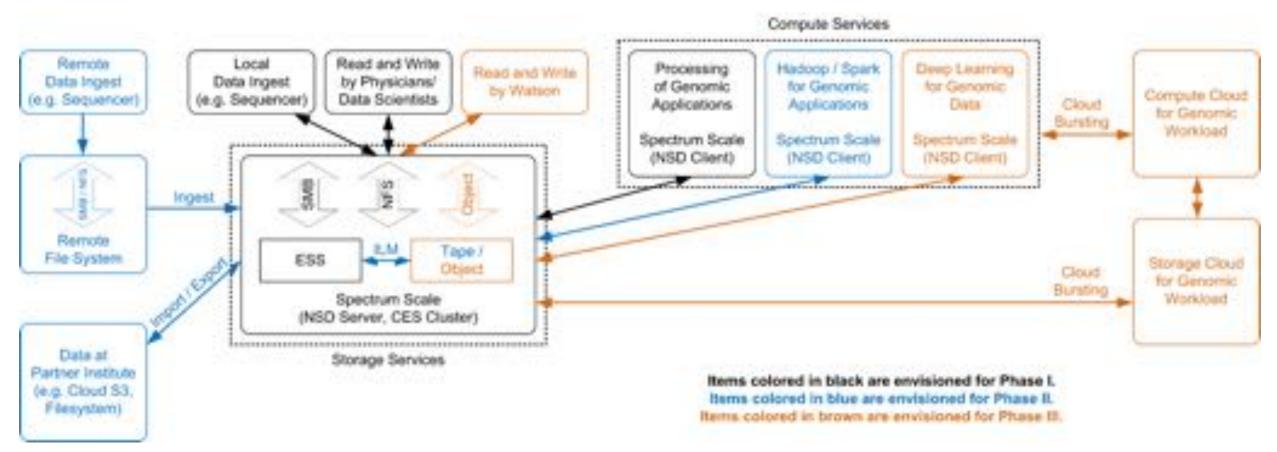
Capabilities - Blueprint V1.1 - Private Network Services

- To integrate all components of the Compute Services and all components of the Storage Service into an IT Infrastructure Solution for Genomics Workload the Private Network provides:
 - A High-Speed Data Network for fast and secure access to genomics data:
 - Storage Nodes are configured with high availability by default (at least two links).
 - **Compute Nodes** are optionally configured with high availability (one or two links).
 - A **Provisioning Network** for provisioning and in-band **management** of the storage and compute components and for **administrative login**.
 - A Service Network for out-band management and monitoring of all solution components.
 - A Scalable Design that can start from a small starter configuration and grow to a large configuration that consists of hundreds of compute nodes and tens PB of storage.

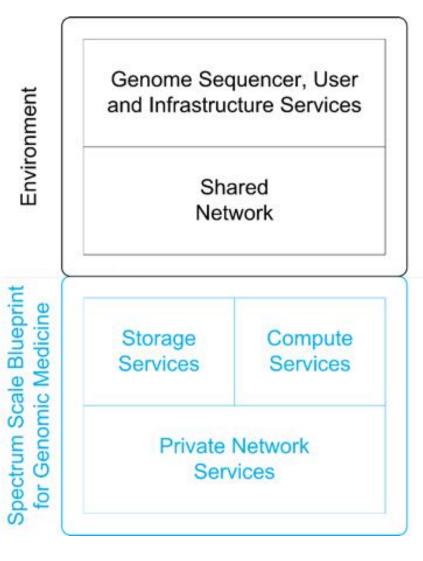
- → Blueprint capabilities have been reviewed with and prioritized by IBM Healthcare and Life Science team.
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Staged Approach

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Composable Building Blocks



The Spectrum Scale Blueprint for Genomics Medicine Workload consists of expertly engineered, composable building blocks which include:

- **best practices guides** for architecture and configuration settings,
- runbooks which describes how to install, configure, monitor and upgrade example configurations,
- **sizing guidelines** which help to define a solution which meets the customers performance requirements,
- deployment workshop with client to customize solution to client's specific needs,
- sales material which enable seller to identify opportunities and create winning proposals,
- a war room where sellers and architects get easy access to subject matter experts.

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