

Storage, HPC, and Enterprise Networking as Local Convergence Points for Scientific Computing

Converged IT Infrastructure In Life Science

Who are we?

Aaron Gardner

Senior Scientific Consultant

Computer engineer who spent the last 15 years with
biologists in situ

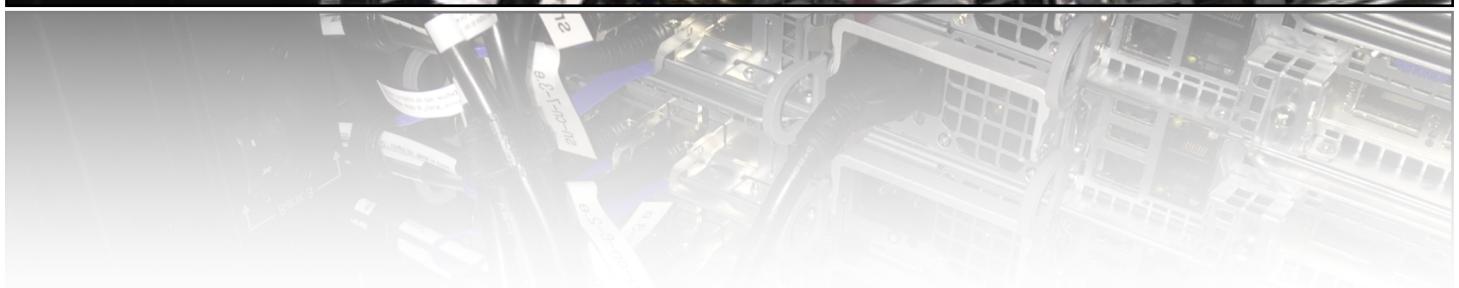
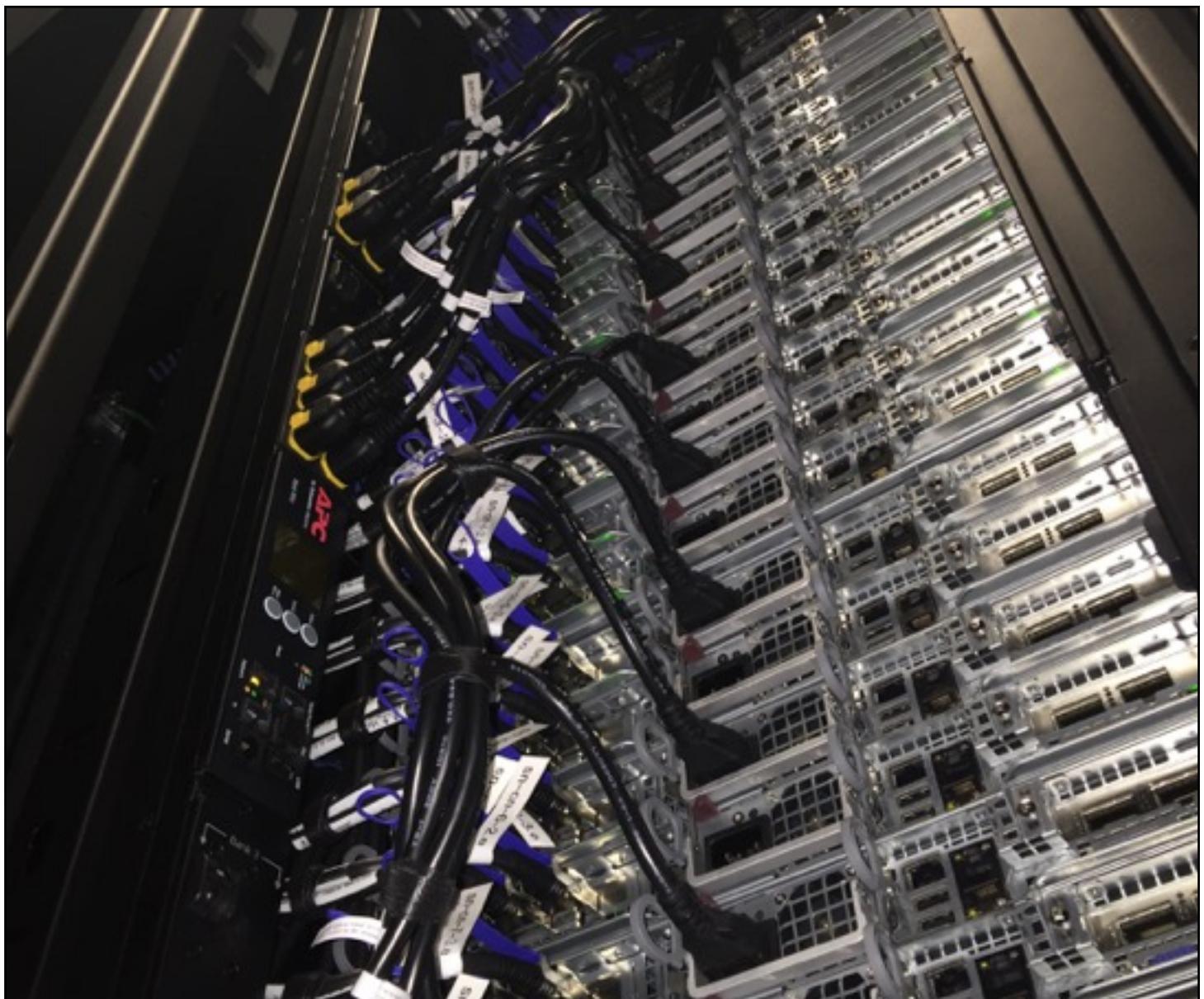
Along the way learned bioinformatics, data
management, HPC, research cyberinfrastructure

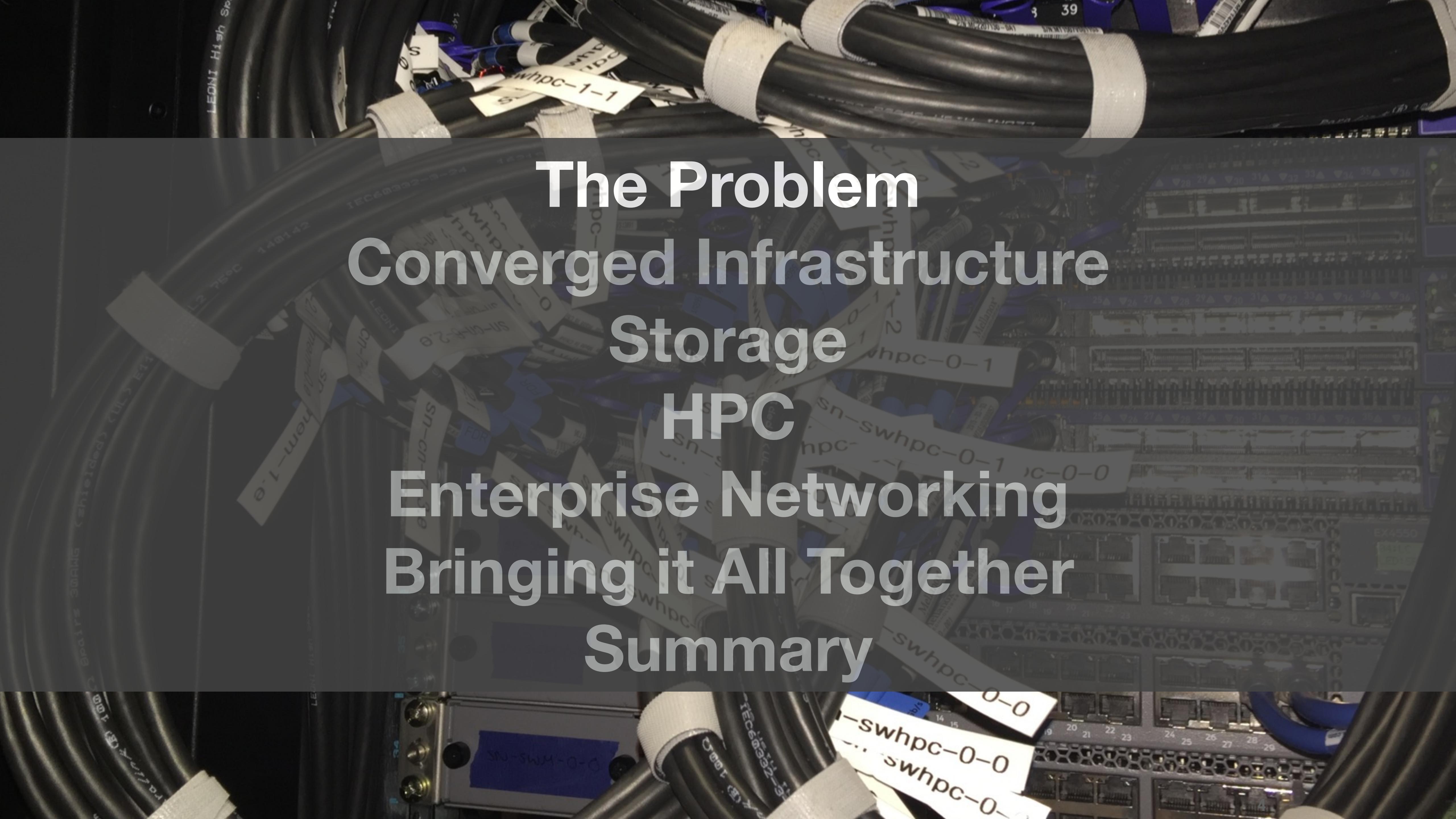
I help enable science!

BioTeam

Who are we?

- ▶ **Independent consulting shop**
- ▶ **Staffed by scientists forced to learn IT, SW & HPC to get our own research done**
- ▶ **13+ years bridging the “gap” between science, IT & high performance computing (HPC)**
- ▶ **BioTeam@BioIT’15**
- ▶ **HPC Trends in the Trenches 2015**
 - ▶ Chris Presents @ 11AM Weds
 - ▶ Lots going on at the conference this year
 - ▶ Come visit us @ booth #357



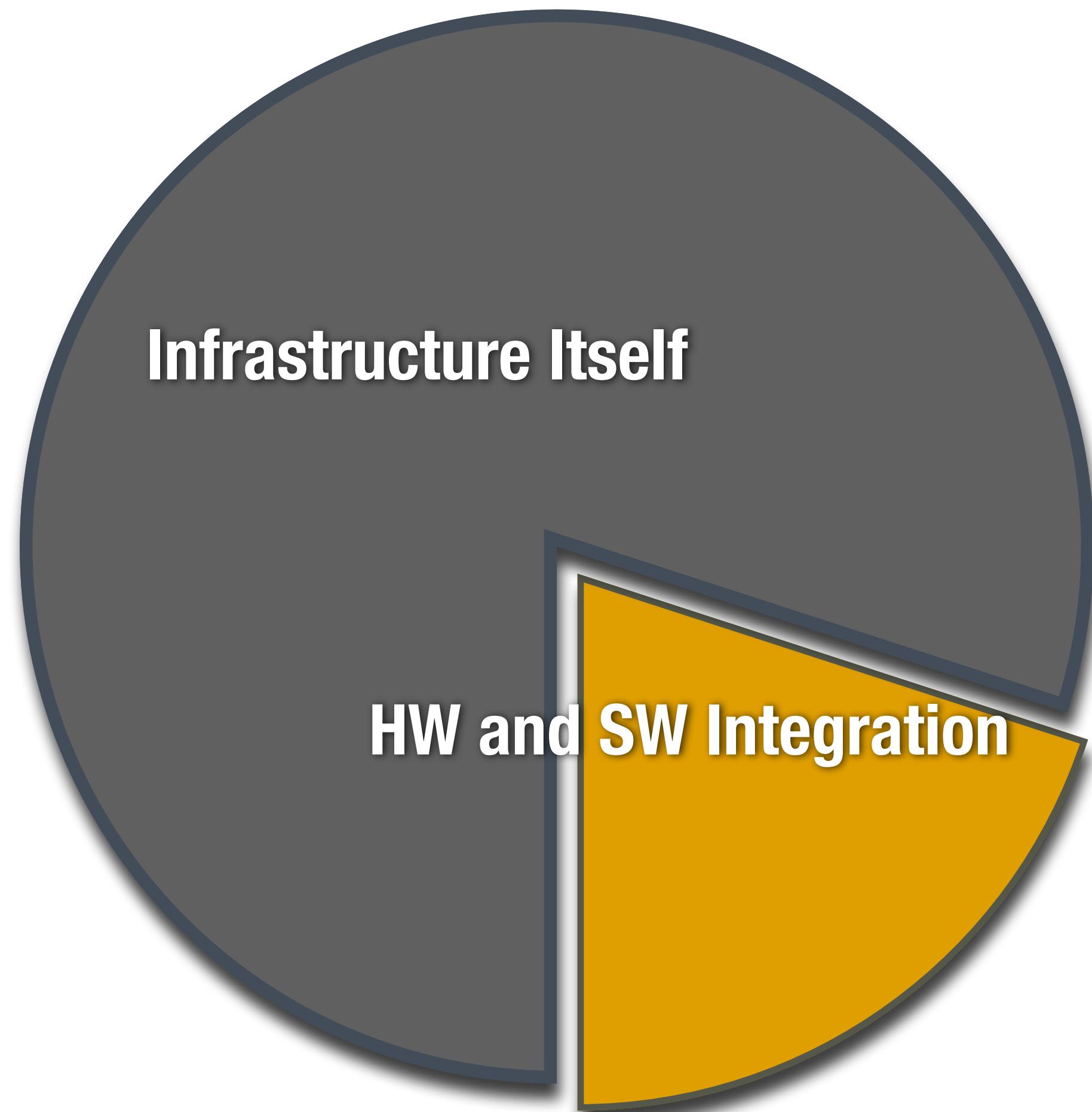


The Problem Converged Infrastructure Storage HPC Enterprise Networking Bringing it All Together Summary

Observation

Research Infrastructure

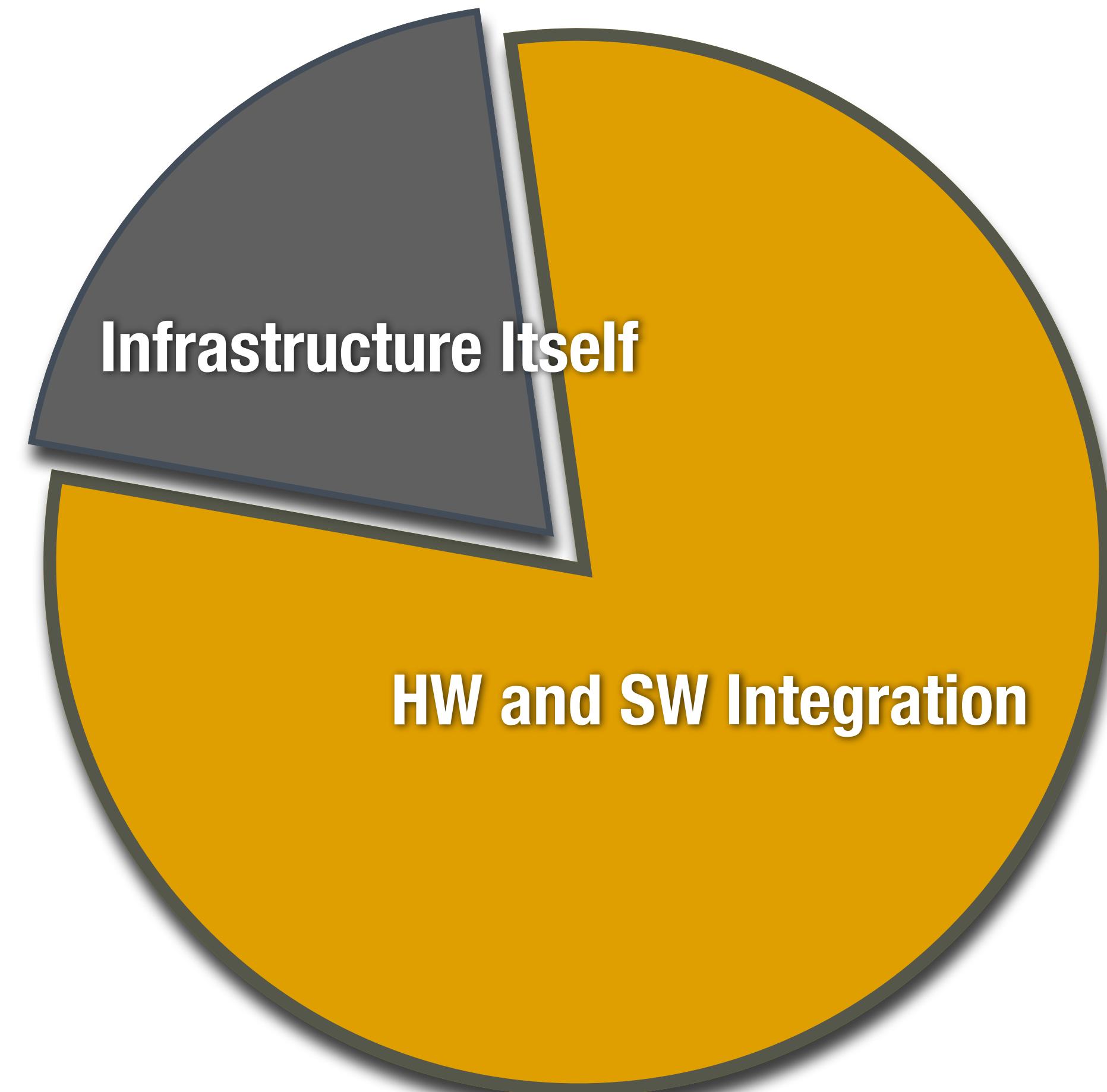
Spending (in theory)...



Observation

Research Infrastructure

Spending (in practice):





Problem: Integration Overhead

Integration Overhead

Research Infrastructure Spending

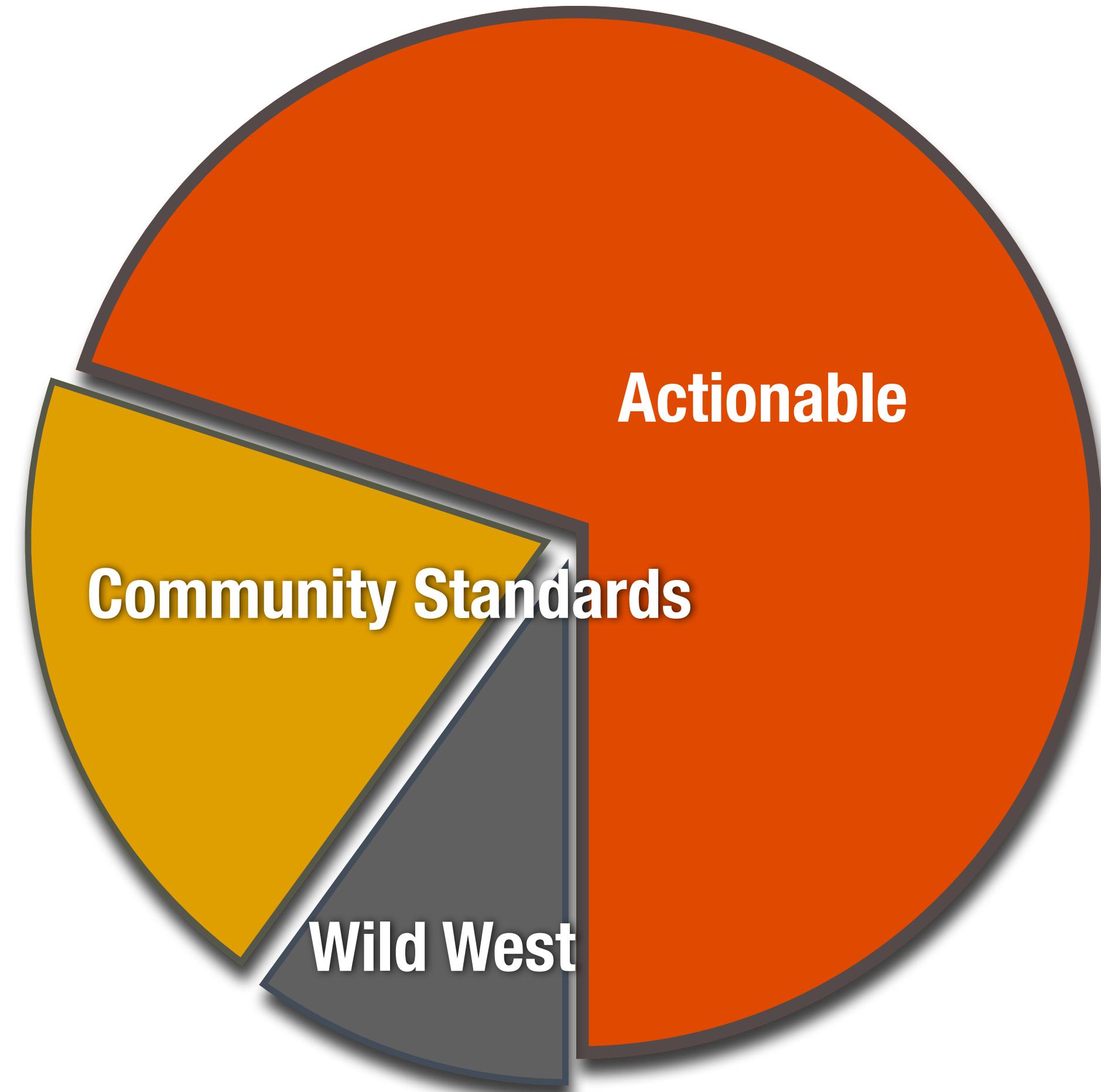
Balancing integration overhead is one of the principal challenges in designing computing environments for biomedical research

- ▶ **True in life sciences as well as other domains**
- ▶ **Building from a parts list never previously integrated**
(stops sounding exciting after you've done it)
- ▶ **Even worse – choices made by choosing from a business portfolio instead of technical merit and efficiency**
(for small and midsize infrastructures, integration overhead balloons)

Observation

Data Analysis for in the Life Sciences

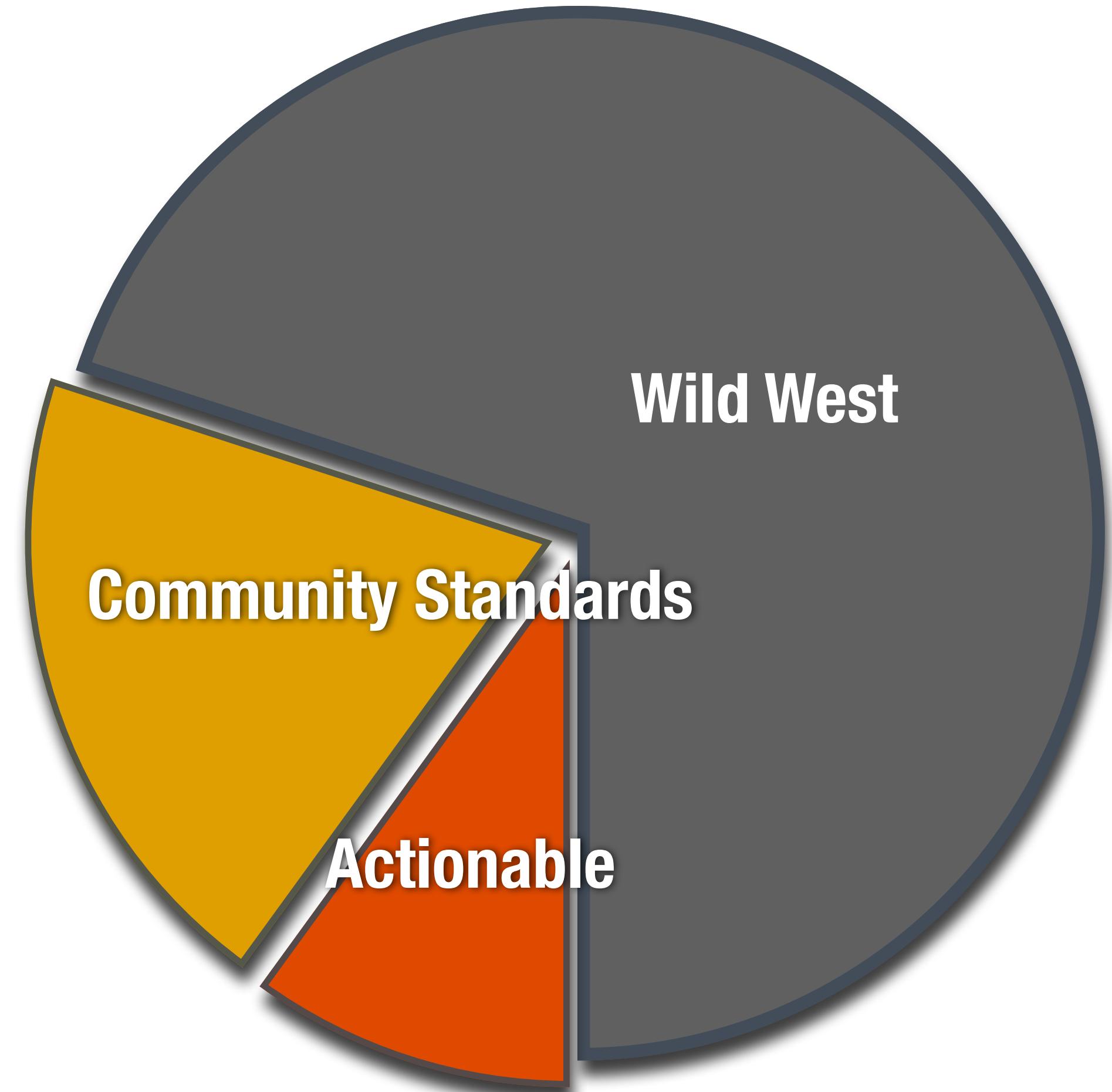
What we are shooting for (in theory)...



Observation

Data Analysis for the Life Sciences

Where we seem to be (in practice):





Problem: Technology Bottleneck

Technology Bottleneck

Data Analysis for Personalized Medicine

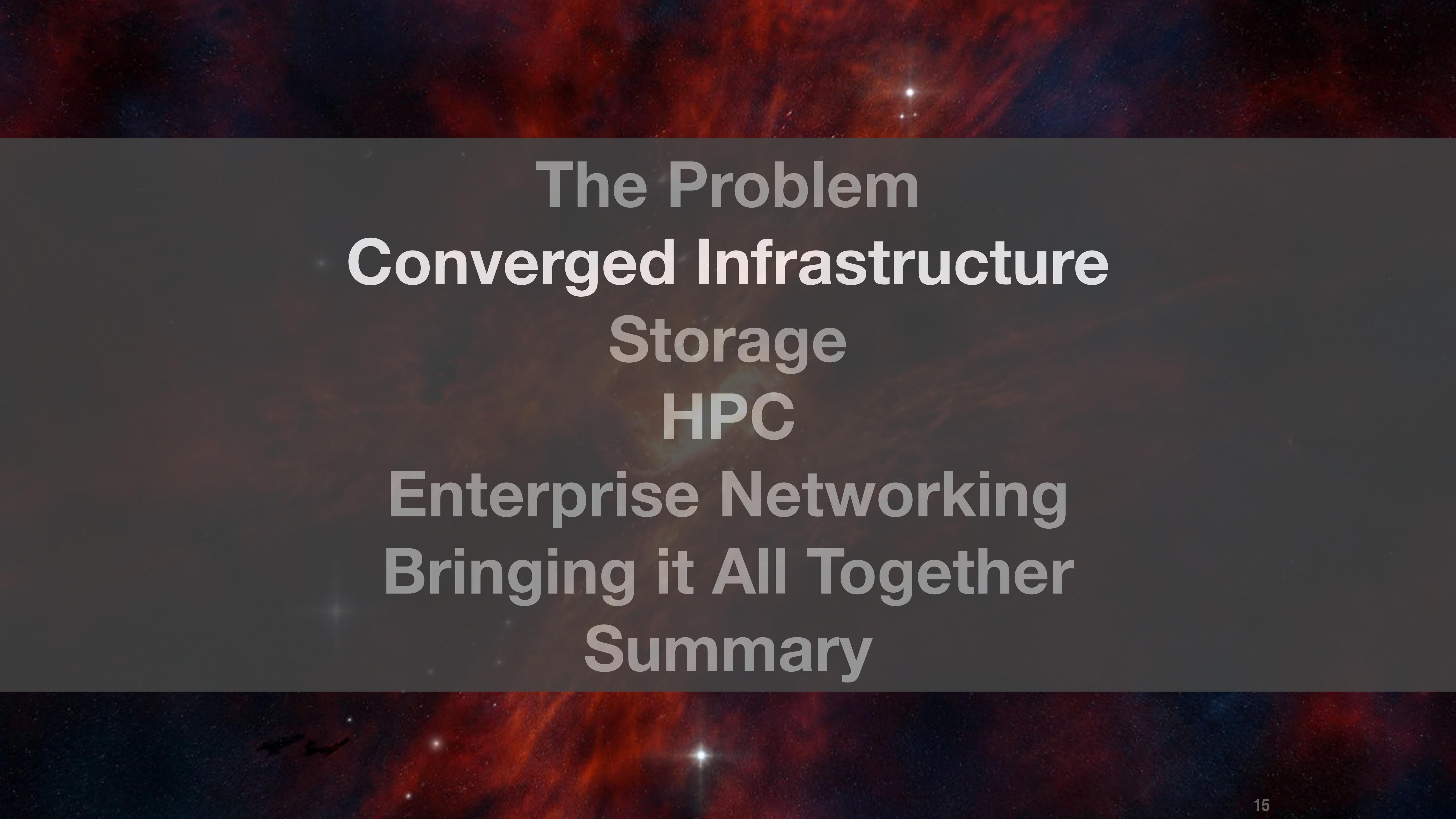
- ▶ **Transition from the information age to the analytics age**
(interpretation of big ludicrous data drives discovery)
- ▶ **Interpretation methods and algorithms in constant flux**
(optimize: wild west → community consensus → actionable)
- ▶ **HPC ranges from difficult to impossible for clinicians to use**
(need the usability and agility of web & mobile with the power of HPC)
- ▶ **Disparate + regulated = hindered collaborations**

“Flakey” Infrastructure

“Flakey” Infrastructure

What is it?

- ▶ **Comprised of separate hardware and software components**
(often purchased several years apart, by different teams)
- ▶ **Pieced into one-off solutions, integrated and tuned on-site**
(at this point they begin generating their own folklore)
- ▶ **As they go through their lifecycle they become snowflakes**
(some turn out well, others are...)



The Problem
Converged Infrastructure
Storage
HPC
Enterprise Networking
Bringing it All Together
Summary

Converged Infrastructure

What is it?

Multiple hardware & software components are developed, selected, integrated, and tuned together, producing a pre-optimized solution
(can be converged, hyper-converged, ludicrous-converged)

- ▶ **Pieces are chosen based on technical merits**
- ▶ **Provided as infrastructure building blocks and appliances**
- ▶ **Organization's talent can now stop (re)integrating HW and SW, they are now free to build software and services**
(stop reintegrating and start adding value)

Life science needs converged solutions!



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BioTeam Pays Attention to Storage

And some of what we have seen isn't pretty

- ▶ **Organizations Drowning in Complexity**
 - ▶ More storage system types and vendors than I have fingers
 - ▶ Making it all work together nearly impossible, brittle
 - ▶ PB+ of misconfigured storage unable to handle small loads
- ▶ **At the small and midsize scale (<5PB)**
 - ▶ More important than ever to know whether you are
 - (1) researching storage or**
 - (2) using storage for research**
 - ▶ **Building your own Petascale storage is still nontrivial**

Headed Toward Converged Model

Quick Litmus Test

Things to Look for in Converged Storage

- ▶ **It should take care of the storage servers and major configuration for you**
 - ▶ Tuning for workload still applies, but vendors should help
- ▶ **Sold such that you just add scalable units**
- ▶ **Tiers are usually pre-integrated by vendors**
- ▶ **Run your own workloads easily**
- ▶ **Your configuration has been baked before**

Emerging Converged Tiered Model

What we are seeing out there more and more...

Tier 0

- ▶ **Burst buffer and/or IOP SSD cache tier**
 - ▶ Reorders IO from large number of clients
 - ▶ Examples: DSSD (EMC), IME (DDN)
 - ▶ Optional but encouraged, critical in larger environments

Emerging Converged Tiered Model

What we are seeing out there more and more...

Tier 1

- ▶ **Distributed Parallel Storage Tier**
 - ▶ Predominantly GPFS and Lustre
 - ▶ Other emerging but it takes a while to bake a FS
 - ▶ Examples: ClusterStor (Seagate), SFA (DDN)
 - ▶ If you get anything to drive HPC you get this tier
 - ▶ Scale out NAS is difficult to leverage for HPC

Emerging Converged Tiered Model

What we are seeing out there more and more...

Tier 2

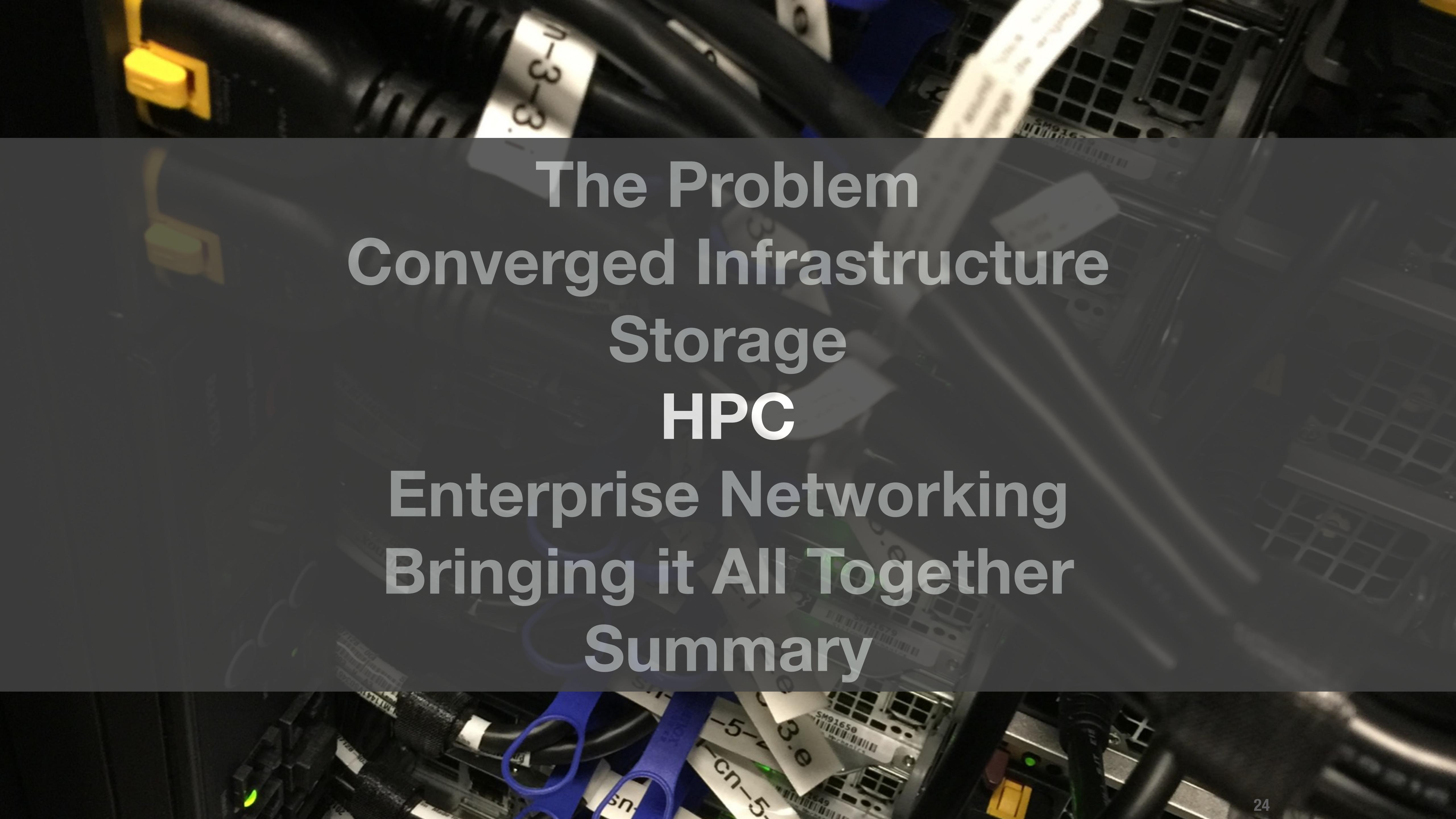
- ▶ **Archival Tier**
 - ▶ Increasingly object storage based
 - ▶ On premise or in public cloud
 - ▶ Sometimes reuse existing scale out NAS investment
 - ▶ Sometimes also fronted by NAS heads (example: Avere)
 - ▶ Use policy engines for movement
 - ▶ GPFS HSM, Lustre Robinhood

Data Lifecycle Management

Control your data

iRODS, the Integrated Rule-Oriented Data System

- ▶ A project for building the next generation data management cyberinfrastructure.
- ▶ iRODS provides a system that enables a flexible, adaptive, customizable data management architecture.
- ▶ Suitable for preserving data over its lifecycle.



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History and Trends - Converged HPC

Setting the scene

- ▶ **Cisco UCS - Early during this wave**
 - ▶ Converged network and compute
- ▶ **Lots of companies entering the market or rebranding last couple of years**
 - ▶ Dell, VMware EVO:RAIL, etc.
 - ▶ NIMBOXX, Nutanix
- ▶ **Difficult to find ones who blend cloud with true HPC hardware**
 - ▶ Example: Onyx OpenStack building blocks

History and Trends - Converged HPC

Setting the scene

- ▶ **HPC nodes used more and more for private cloud too**
- ▶ **Requires versatility in the building blocks**
- ▶ **Technologies that enable SR-IOV, software defined networking, etc. more important now for HPC**
- ▶ **Lately compute has been seen as the “easy” part, and a commodity**
 - ▶ While still true, more and more vendors are now beginning to bring compute into their converged portfolio, even in HPC context

History and Trends - Converged HPC

Setting the scene

- ▶ **In converged designs, homogeneous node types are what we usually look for**
 - ▶ Easier to scale uniformly for power, density, workload
- ▶ **For HPC in the life sciences, recommend having high memory building blocks, accelerator building blocks, etc.**
 - ▶ The benefits these node types offer outweigh the simplicity of a single compute node type

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The Problem Converged Infrastructure Storage HPC Enterprise Networking Bringing it All Together Summary

To Converge or Not to Converge?

Is Converged Infrastructure in Your Critical Path?

Not as necessary when:

- ▶ **Hiring lots of smart people and committing their time to infrastructure**
- ▶ **Attacking a single or small set of large problems**
- ▶ **Rarely revalidating or reintegrating your HW stack after deployment**



To Converge or Not to Converge?

Is Converged Infrastructure in Your Critical Path?

Tie your platform closely to mixed hardware stack and...

- **Increased staff time to reintegrate or revalidate**
- **Increased time to rewrite code for new architectures**
- **Decreased legacy and vendor-controlled codes**
- **Decreased infrastructure flexibility**
- **Decreased ability to handle yet unknown and unsolved problems**

Tiered Service Model

Change Staff Roles

- ▶ **DevOps and the cloud have changed the relationship between the researcher and the IT practitioner permanently**
- ▶ **Research computing staff should be developing best practices, not acting as a human ‘sudo’ for informaticists, etc.**

Solution: Move to a tiered service and support model

Tiered Service Model

Change Staff Roles

1

Users instantiate **resources** on demand which they have **privileged** access to—but no support is offered beyond clearing hang-ups



2

Services requiring a higher degree of reliability and/or security are built and managed by IT staff, with unprivileged access provided to users



3

Core computational services are still supported end-to-end by IT staff, and are consumed by resources in the previous two levels

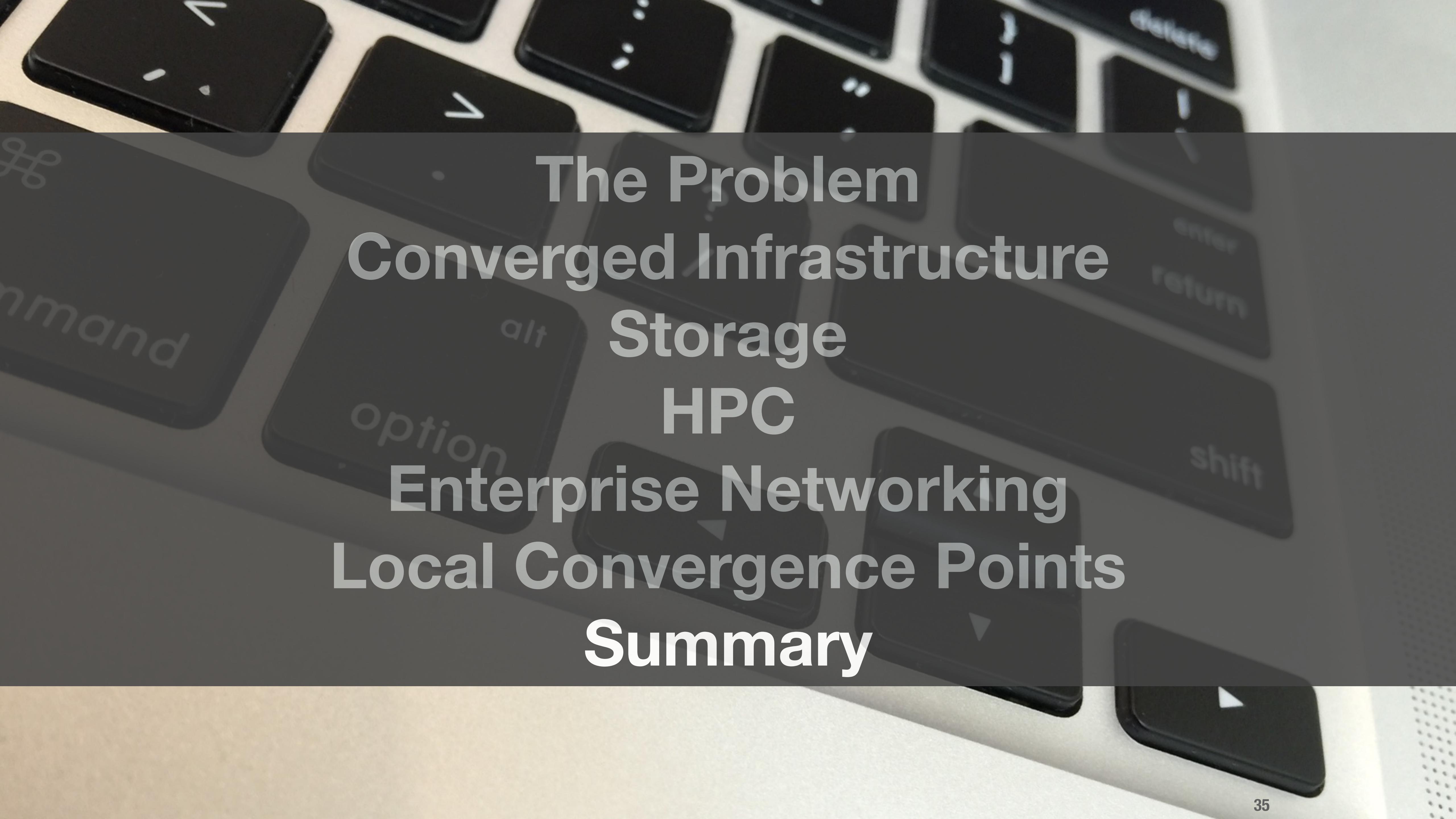


Tiered Service Model

Changing Staff Roles

Challenges With This Model:

- ▶ Need single instance resources capable of dealing with large data
- ▶ Now need multitenancy capabilities even as a single organization
- ▶ Minimize latency to better utilize limited resources
- ▶ And public cloud's massive scalability approach might not be suitable for small or midsize environments with legacy codes, inexperienced users, etc.



The Problem Converged Infrastructure Storage HPC Enterprise Networking Local Convergence Points Summary



The Freedom to Discover



Thank You; Questions and Discussion Welcome