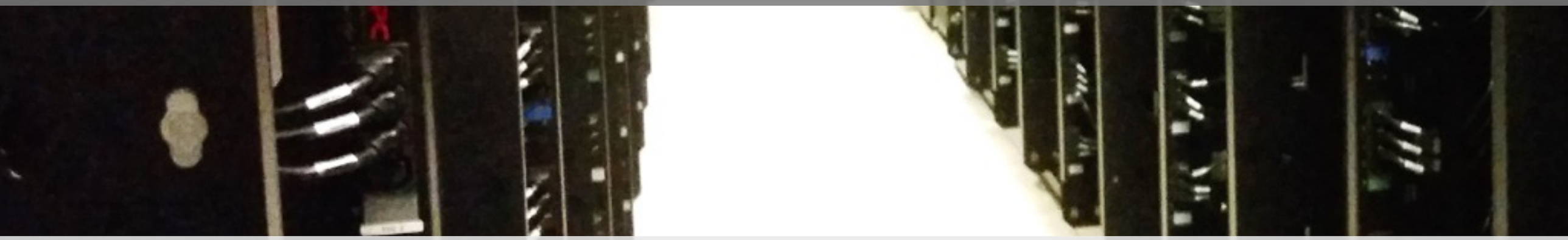
# Converged IT Infrastructure in Life Sciences

*Org Challenges, Networks, and Science DMZs, Oh My!*



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**BioIT World Converged IT Workshop - 2015**

# We've noticed a few things

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We have a unique perspective across much of life sciences

- **Big Data has arrived in Life Sciences**
- **Data is being generated at unprecedented rates**
- **Research and Biomedical Orgs were caught off guard**
- **IT running to catch up, limited budgets**
- **Money is tight, Orgs reluctant to invest in Bio-IT**

**25% of all Life Scientists will require HPC in 2015!**

# Research is hard

It's being made harder by lack of support and infrastructure that works for them

- **Scientists are getting frustrated**
- **Stubborn, fight for what they need**
- **They will build a cluster under their desk if it gets the job done**
- **In general they will win against IT, eventually**

# Big Picture / Meta Issue

- **HUGE revolution in the rate at which lab platforms are being redesigned, improved & refreshed**
- **IT not a part of the conversation, running to catch up**

# The Central Problem Is ...

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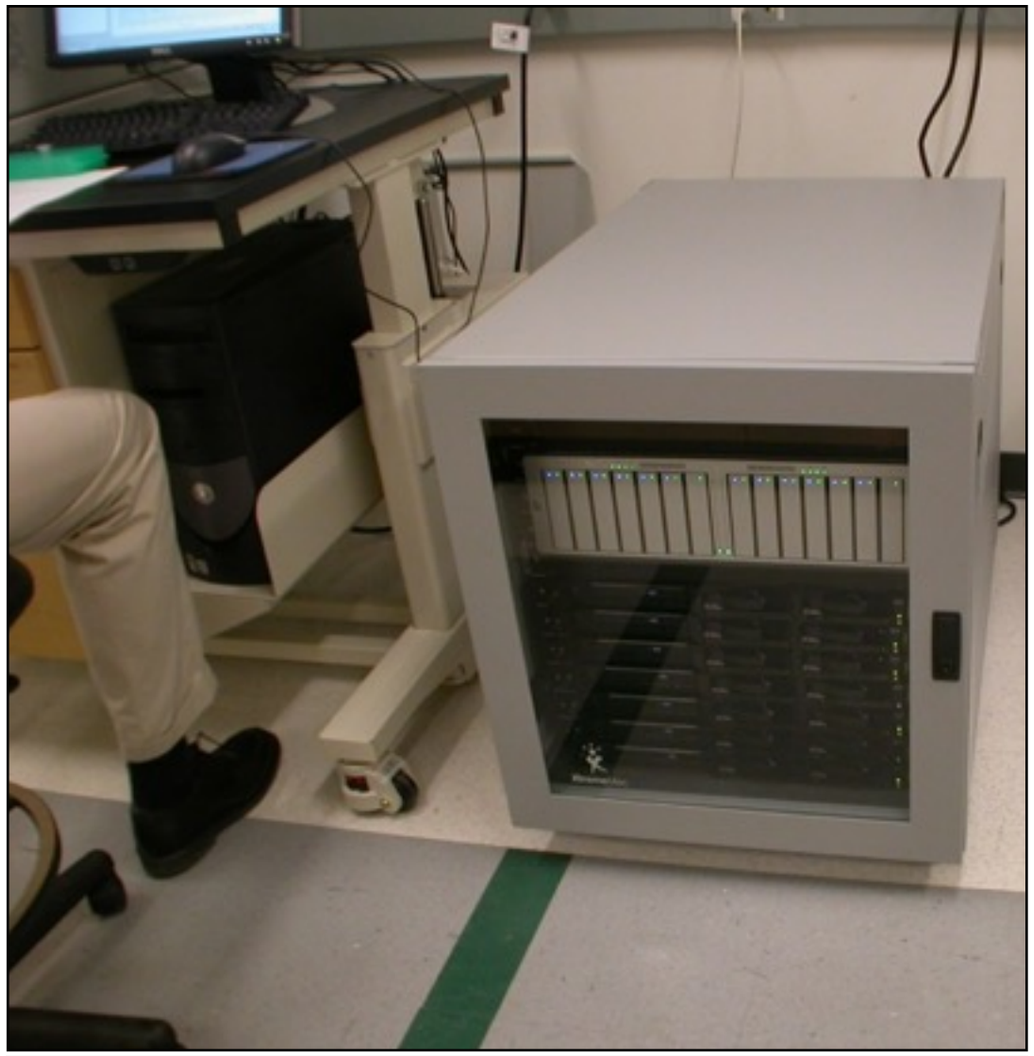
Science progressing way faster than IT can refresh/ change

- **Instrumentation & protocols are changing FAR FASTER than we can refresh our Research-IT & Scientific Computing infrastructure**
  - Bench science is changing month-to-month ...
  - ... while our IT infrastructure only gets refreshed every 2-7 years
- **We have to design systems TODAY that can support unknown research requirements & workflows over many years (gulp ...)**

# The Central Problem Is ...

- The easy period is over
- 5 years ago - under the desk solutions worked
- This doesn't work any more!



# The new normal for informatics

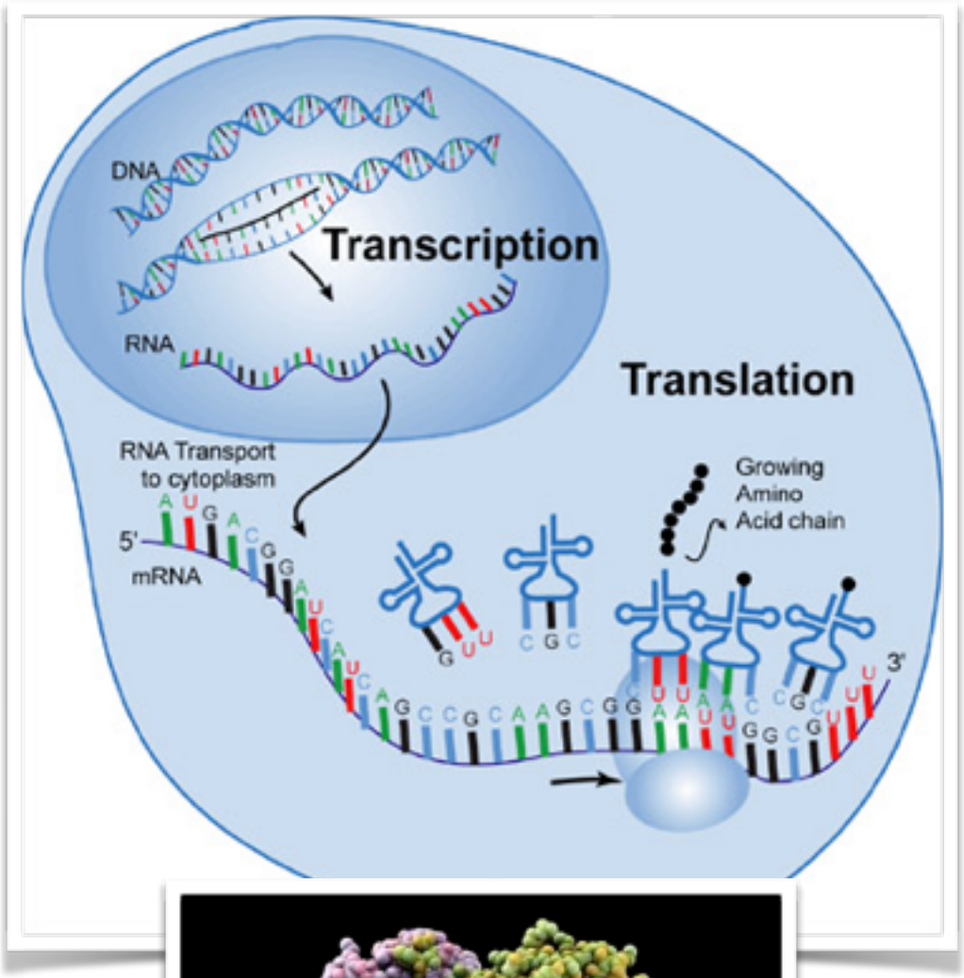
# What are the drivers in Bio-IT today?

# Genomics: Next Generation Sequencing (NGS)

# The big deal about DNA

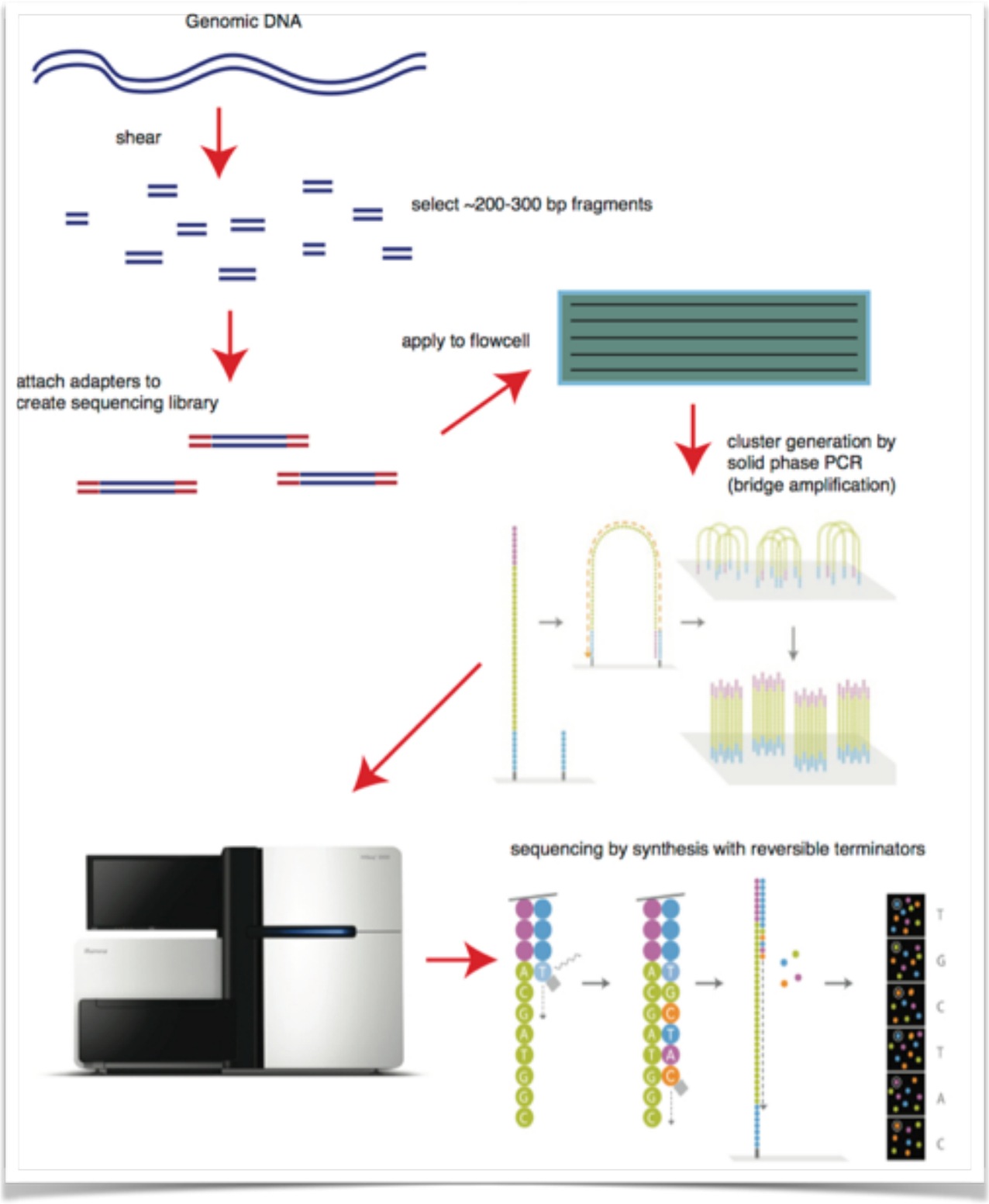
## It's like the hard drive of life

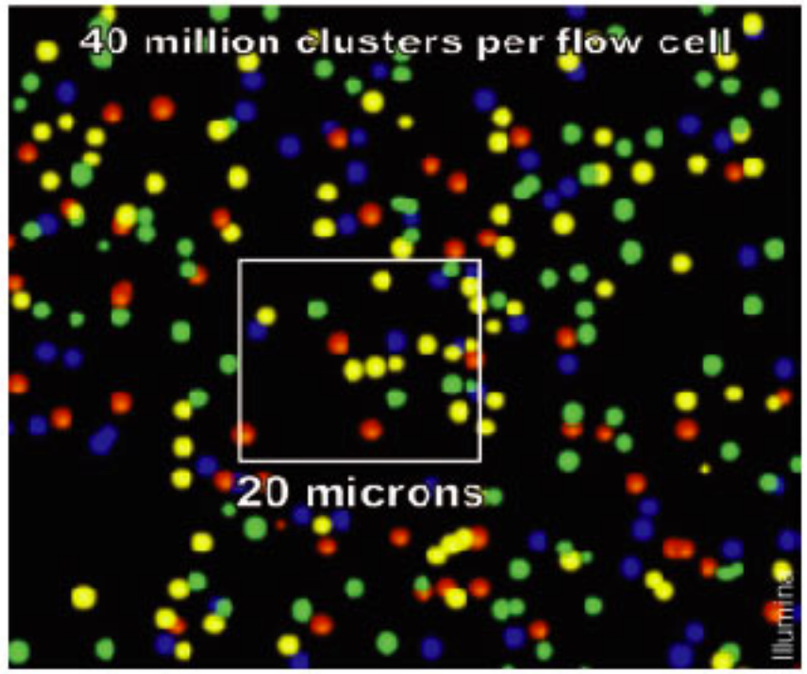
- **DNA is the template of life**
- **DNA is read --> RNA**
- **RNA is read --> Proteins**
- **Proteins are the functional machinery that make life possible**
- **Understanding the template = understanding basis for disease**




# How does NGS work?

## Sequencing by Synthesis




# How does NGS work?

## Reference assembly, variant calling

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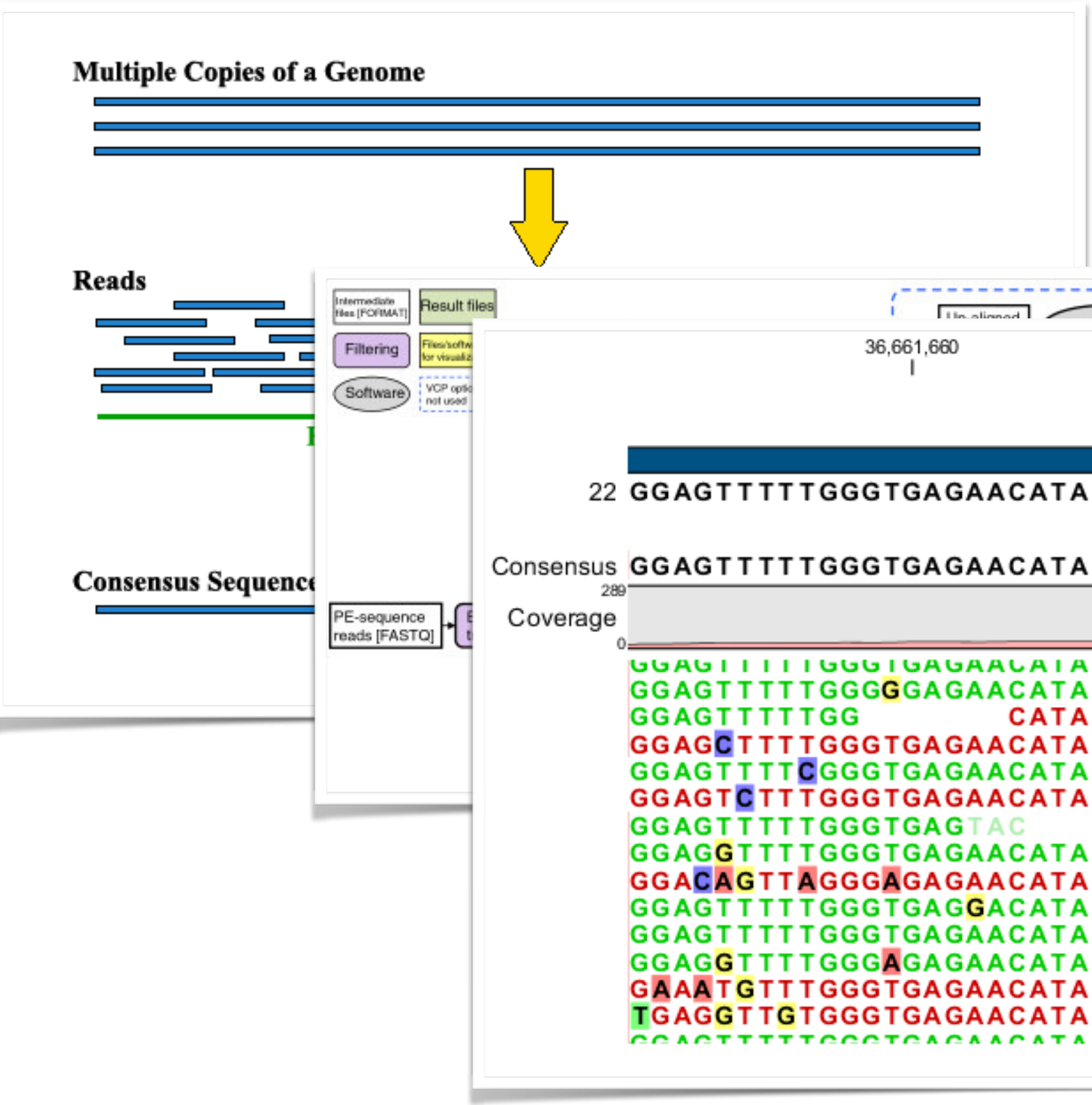

# The Human Genome

## Gateway to personalized medicine

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- **3.2 Gbp**
- **23 chromosomes**
- **~21,000 genes**
- **Over 55M known variations**

# The Problem...

...and why NGS is the primary driver

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- **Sequencers are now relatively cheap and fast**
- **Some can generate a human genome in 18 hours, for $2,000**
- **Everyone is doing it**
- **Can generate 3TB of data in that time**
- **First genome took 13 years and $2.7B to complete**

# Other Methodologies Not Far Behind

# High-throughput Imaging

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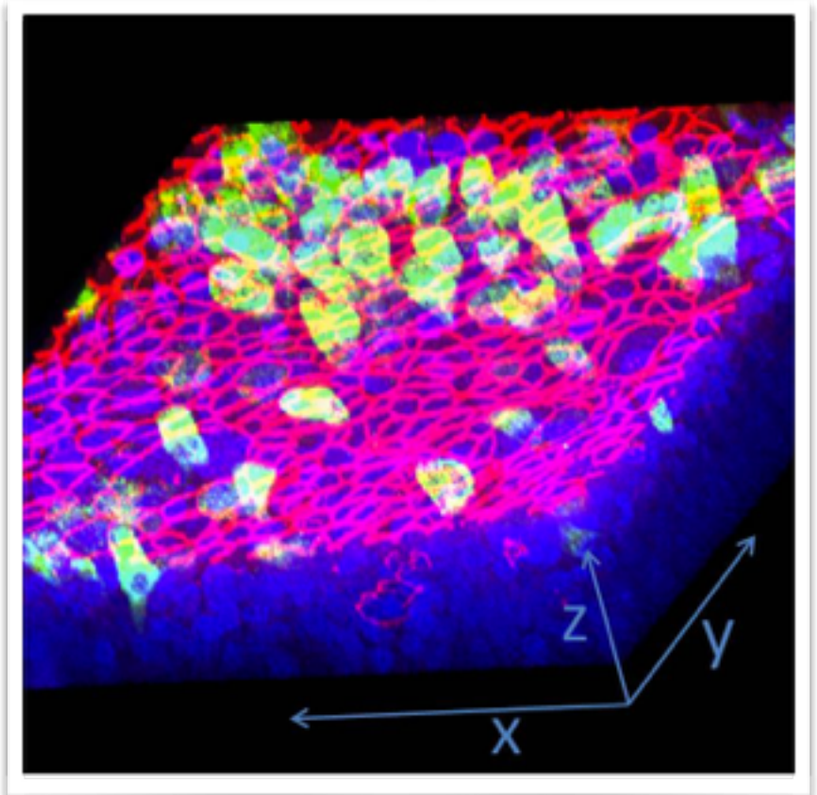
- **Robotics screening millions of compounds on live cells 24/7**
  - Not as much data as genomics in volume, but just as complex
  - Data volumes in the 10's TB/week
- **Confocal Imaging**
  - Scanning 100's of tissue sections/ week, each with 10's of scans, each with 20-40 layers and multiple florescent channels
  - Data volumes in the 1's - 10's TB/ week



# High-res medical imaging

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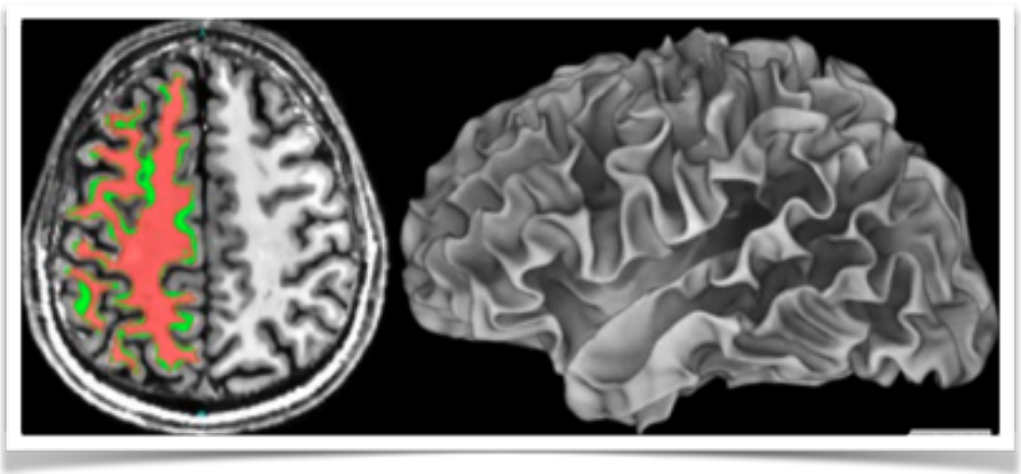
High-power, dense detector MRI scanners in use 24/7 at large research hospitals

- **Creating 3D models of brains, comparing large datasets**
- **Using those models to perform detailed neurosurgery with real-time analytic feedback from supercomputer in the OR (cool stuff)**
- **Also generates 10's of TB/ week**



# This is a huge problem

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- Causing a literal deluge of data, in the 10's of Petabytes
- NIH generating 1.5PB of data/month
- First real case in life science where 100Gb networking might really be needed
- But, not enough storage or compute

# Most common high-speed network: FedEx

# And the problem is getting even bigger

# What to do with all that data?

## Why, giant meta-analyses, of course

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- **Typical problem across all of big data: how do you use it?**
- **In life sciences: no real standards of data formats**
- **Data scattered all over, despite push for Data Commons**
- **Not always accessible**
- **Combining the data if you have it all is a real challenge**

# A Compounding Problem...

Scientists don't like to share (really!)

- **The fear:**
  - if someone sees data before it is published, they might steal it and publish it themselves (getting scooped)

- **Causes:**
  - Long time to publication
  - Outdated methods of assigning scientific credit
  - Not properly incentivized

# A Problem for Data Commons

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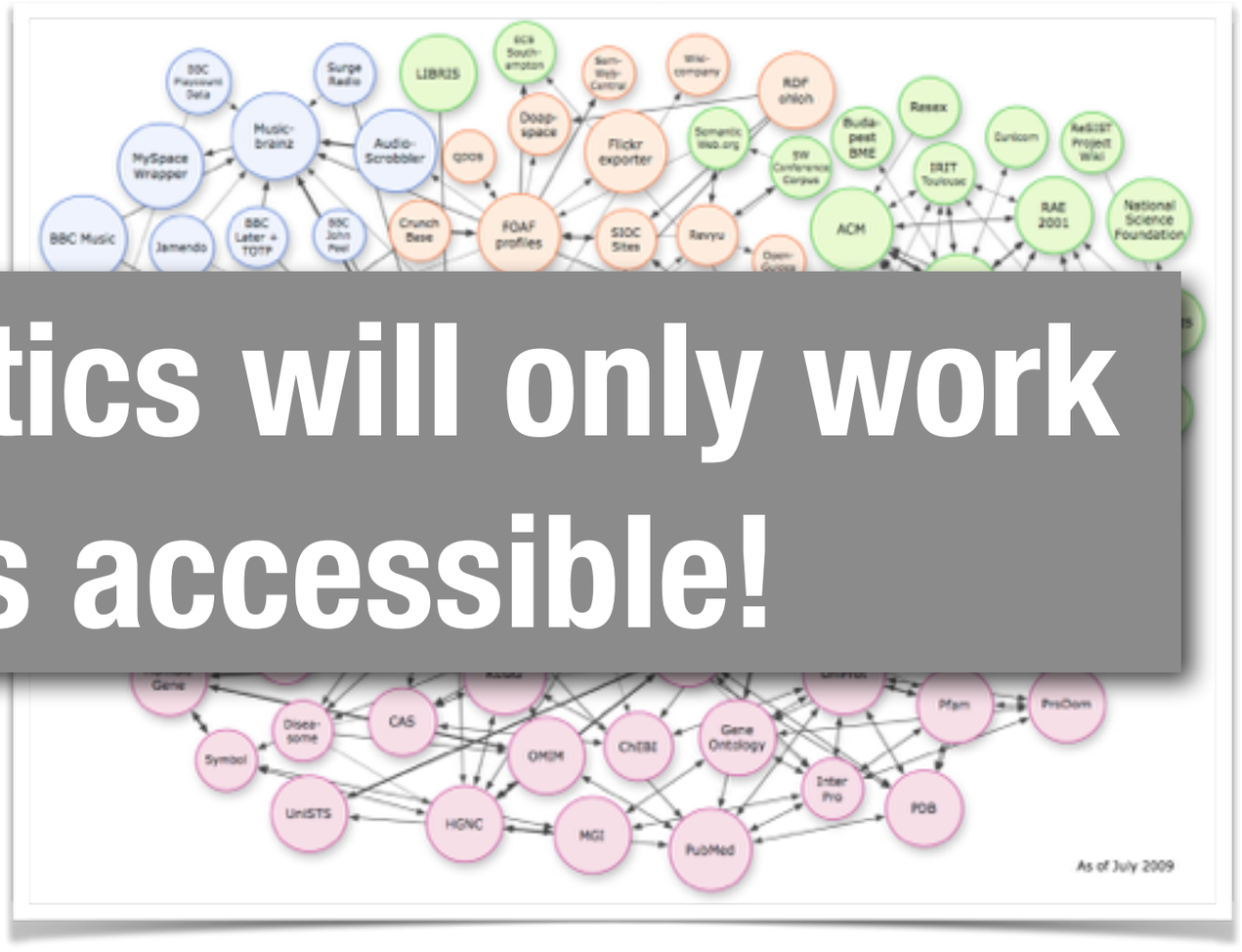
## Sharing required

- **Data piling up**
- **Bad network**
- **Wild-west file formats/algorithms**
- **No sharing**




**Hyperscale analytics will only work if the data is accessible!**

# But wait! There’s more!

# File & Data Types

## We have them all

- **Massive text files**
- **Massive binary files**
- **Flatfile ‘databases’**
- **Spreadsheets everywhere**
- **Directories w/ 6 million files**
- **Large files: 600GB+**
- **Small files: 30kb or smaller**

# Application characteristics

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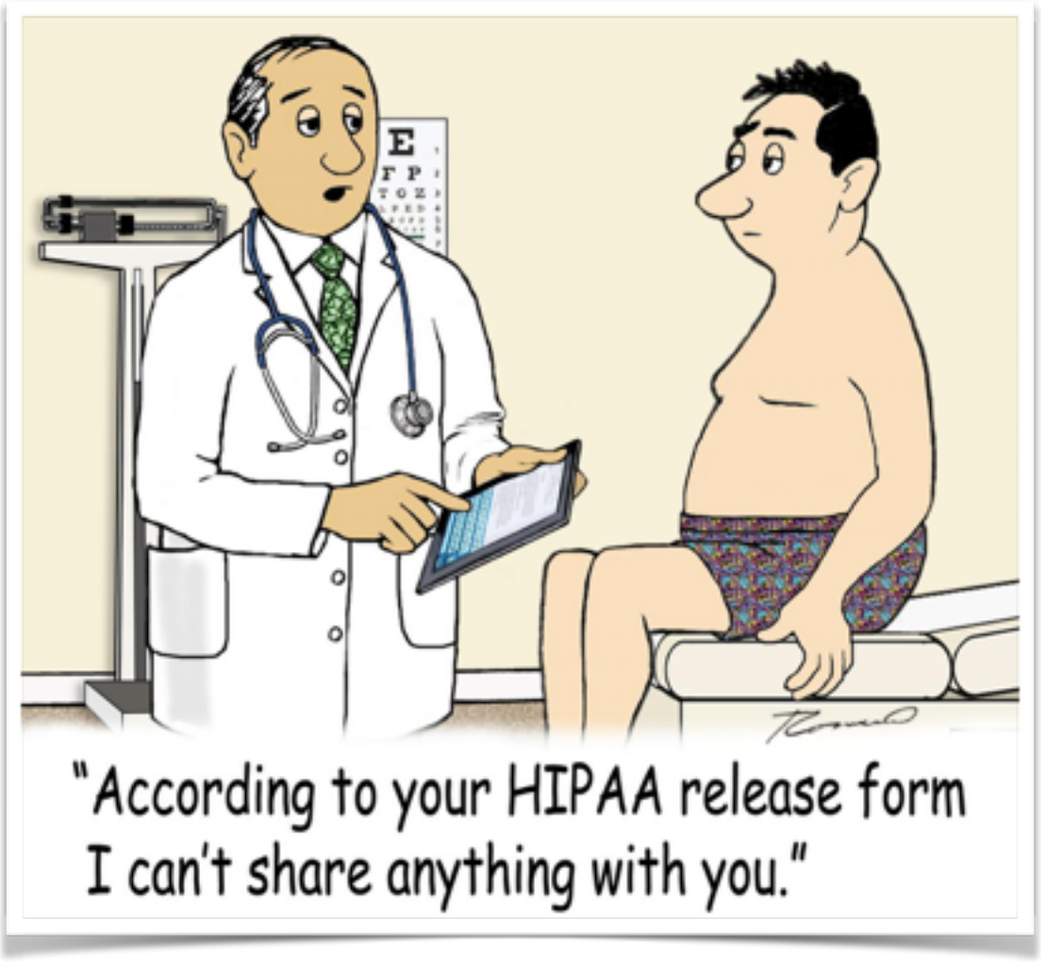
- **Mostly SMP/threaded apps performance bound by IO and/or RAM**
- **Hundreds of apps, codes & toolkits**
- **1TB - 2TB RAM “High Memory” applications (large graphs, genomic assembly)**
- **Lots of Perl/Python/R**
- **MPI is rare**
  - Well written MPI is even rarer
- **Few MPI apps actually benefit from expensive low-latency interconnects***
  - *Chemistry, modeling and structure work is the exception

# Clinical/Regulated more complicated

Need to protect PII, sensitive/confidential information

- **Historically difficult to do**
- **Opposite of the Science DMZ model: compliance at the cost of performance**
- **Deeper security than enterprise, mostly because the SSO and compliance officers don't know better (safest?)**
- **Doesn't work anymore, data generated from clinics and the field increasing rapidly**



# Technologies + regulated data + HPC

# If IT gets it wrong ...

- **Lost opportunity**
- **Missing capability**
- **Frustrated & very vocal scientific staff**
- **Problems in recruiting, retention, publication & product development**

# Successful Bio-IT orgs

IT staff become a part of the research projects

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- **When IT and scientists at the table together, mutual understanding happens**
- **IT is driven to innovate to accommodate science**
- **Scientists better understand resourcing**
- **Roadblocks are removed, science is enabled**

# Build for the Use Case!

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Don’t just build for performance or be sold by vendors

- **Building for hardware is short-sighted**
- **System needs to solve problems, not create more for scientists**
- **Fun to engineer for speed, to buy shiny things, but not terribly useful in LifeSci if it doesn’t solve a problem**
- **That means: take the time to understand the use cases, and design to that. Way more fun in the long-term**

# Life Scientists: Thugs of HPC

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If you have it, they will break it

- **Every kind of file you can imagine**
- **Every kind of algorithm (good, bad, ugly)**
- **Want it all, right now**
- **They keep everything**
- **Don’t want to pay for it**
- **Your health might depend on it (seriously!)**

# Networking in Life Science

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- **May surpass storage as our #1 infrastructure headache**
- **Why?**
  - Petascale storage meaningless if you can't access/move it
  - Enterprise network security usually inhibits research data flow
  - 10-Gig, 40-Gig and 100-Gig networking will force significant changes elsewhere in the 'bio-IT' infrastructure

# Getting Data out of the Laboratory

# Laboratories not Integrated

## Usually very little IT infrastructure in labs

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- **Tons of data generating equipment going in now**
- **Can generate 15GB of data in 50 hours**
- **Others can generate 64GB/day**
- **Labs are not designed to transmit data, lucky if wired for ethernet**

# Getting data out

OK, so write data over ethernet to network drive…

- **Sounds good, 64GB in 24 hours ~= 6Mb/s**
- **Problem: desktop class ethernet adaptors**
- **No error checking, no retries, no MD5, no local buffer**
- **If network goes, whole run is lost**
- **Also, definitely no encryption**

# Getting data out

Clinicians have to get creative, but not in a good way

- **Usually ends up going to local workstation, locked down by IT**
- **Go buy the cheapest disks they can, sometimes encrypted USB disks**
- **Carry it somewhere**
  - Transfer the data to a workstation,
  - Put into compliant database, EHR
  - Not good for analytics
  - HPC use forbidden unless depersonalized, or dedicated HPC

# Lab data transit not huge!

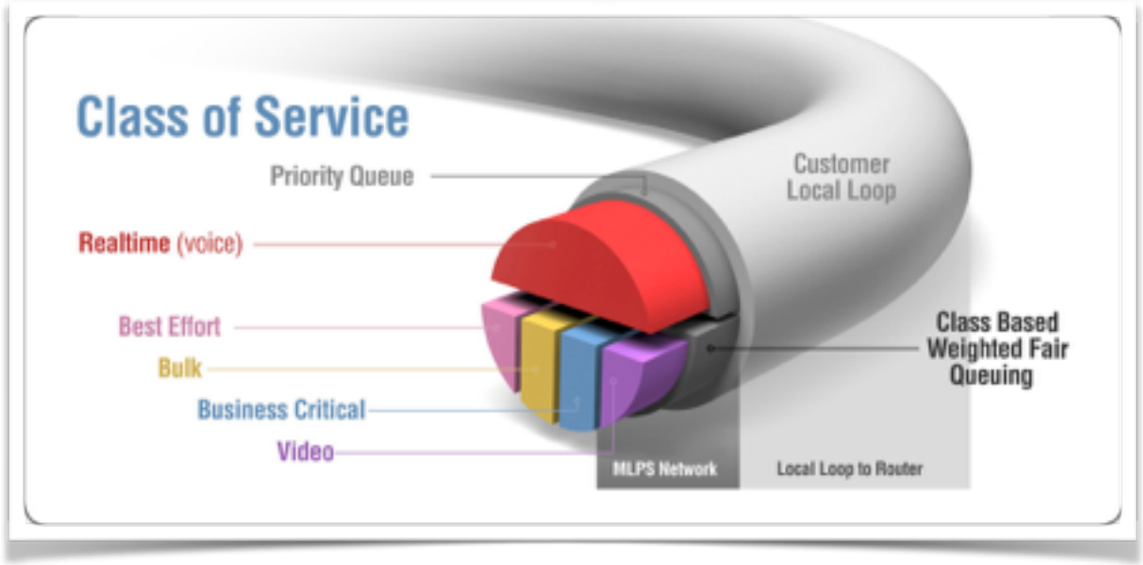
Unless you're dealing with a bigger lab with lots of equipment, or a core facility

- **Fast networking not required, 100Mb OK**
- **Just *GOOD* networking**
- **But!**
  - Collections of data eventually need to be moved for analysis
  - Now you need fast networking
  - Given the problems: how?

# Successful models

Some generalized network models that have successfully solved the problem

- **Most of it is protocol and topology**
- **Quality of Service (QoS)**
- **Appropriate segmentation (L2 and/or L3)**
- **MPLS paths**
- **Intermediate protocols (i.e., Aspera FASP)**
- **One way or another, guarantee transfer**
- **Encrypt the data in flight from data transfer node**



# Storing the Data

# Storage: a networking problem

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As storage needs increase, the need to transmit it goes up too

- **Networking will quickly replace storage as #1 headache in Bio-IT**
- **Petascale storage is useless without high-performance networking**
- **Most enterprise networks won't cut it**

# Storing Clinical Data

Huge problem!

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- **Need isolated storage (usually)**
- **Need data encrypted at rest/in-flight**
- **Keys need to be stored somewhere else secure**
- **Keep PII/PHI safe from espionage at all costs**
- **Usually means you can’t use institutional storage**

# Storage networking: solutions

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## Internal networking more critical than external for petascale storage

- **Infrastructure must be able to support the inevitable 1PB transit**
  - Disaster recovery
  - High-availability
  - Backup
- **Need at least 10Gb**
  - Probably dedicated 10Gb per >1PB storage facility: 40Gb min —> 1Tb backbone
- **1Gb will not cut it for that data size**
  - ~97 days to transmit at saturation
  - 10Gb: ~9.7 days

# Storage networking: solutions

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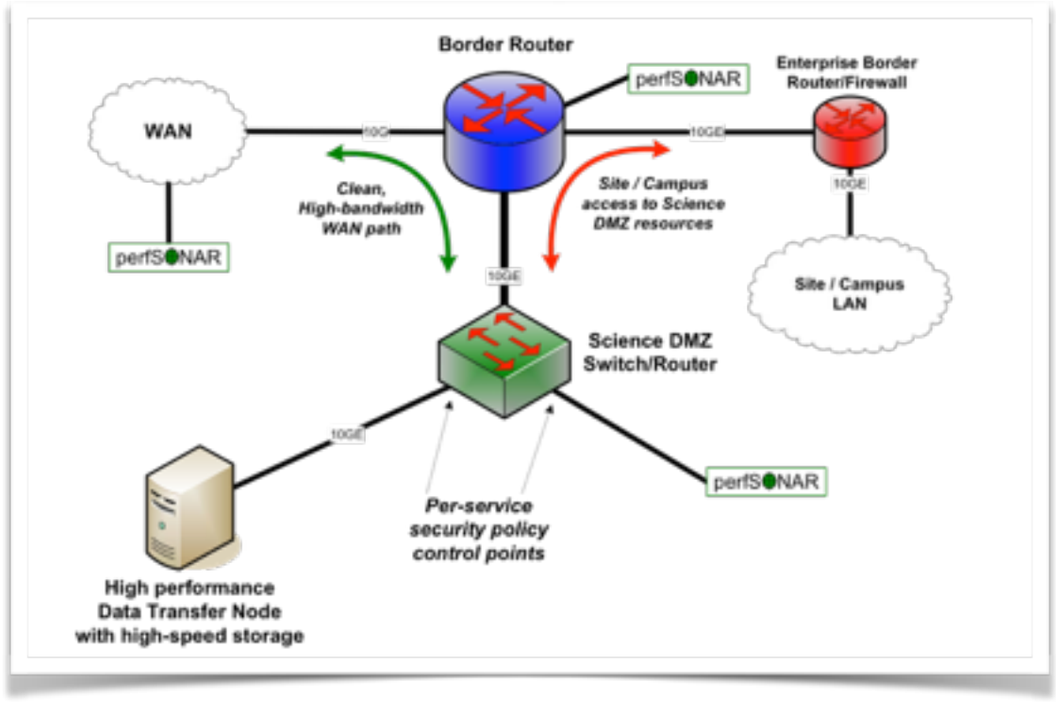
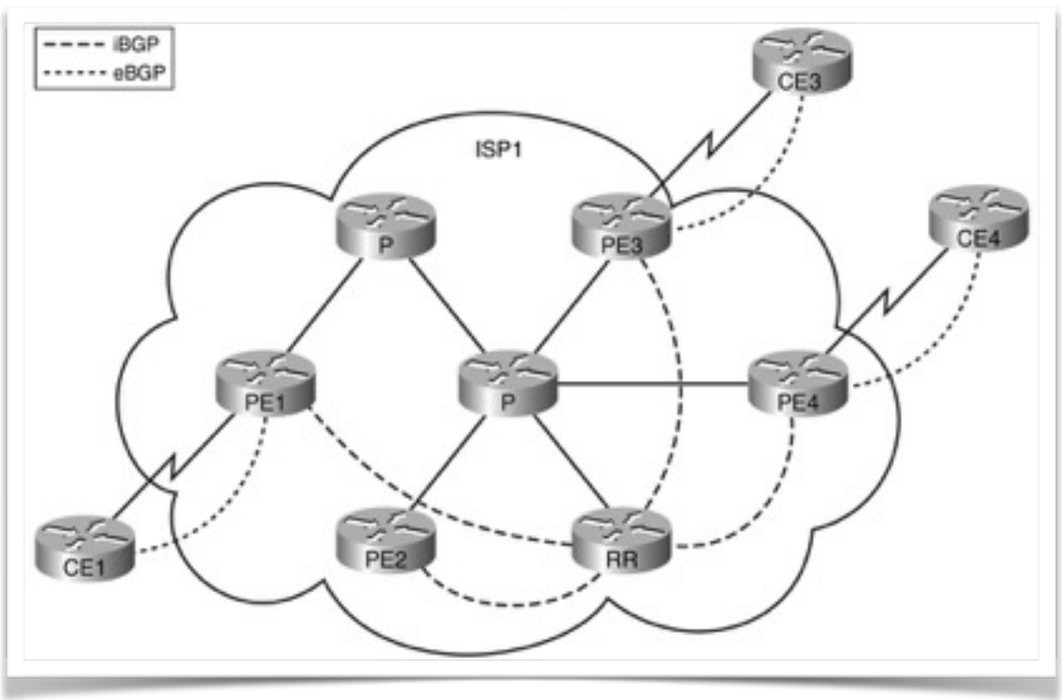
## And now, the real problem: topology and logical design

- **Need a scaling internal topology**
- **One core switch doing all routing and packet transit == bad**
- **More advanced designs needed**
- **Also: prioritize performance over security**
  - Nearly impossible for most orgs
- **Most implemented option: Science DMZ**
- **Additional implementations for segmentation, isolation, filtering, and encryption: small ISP topology very useful for protecting data**



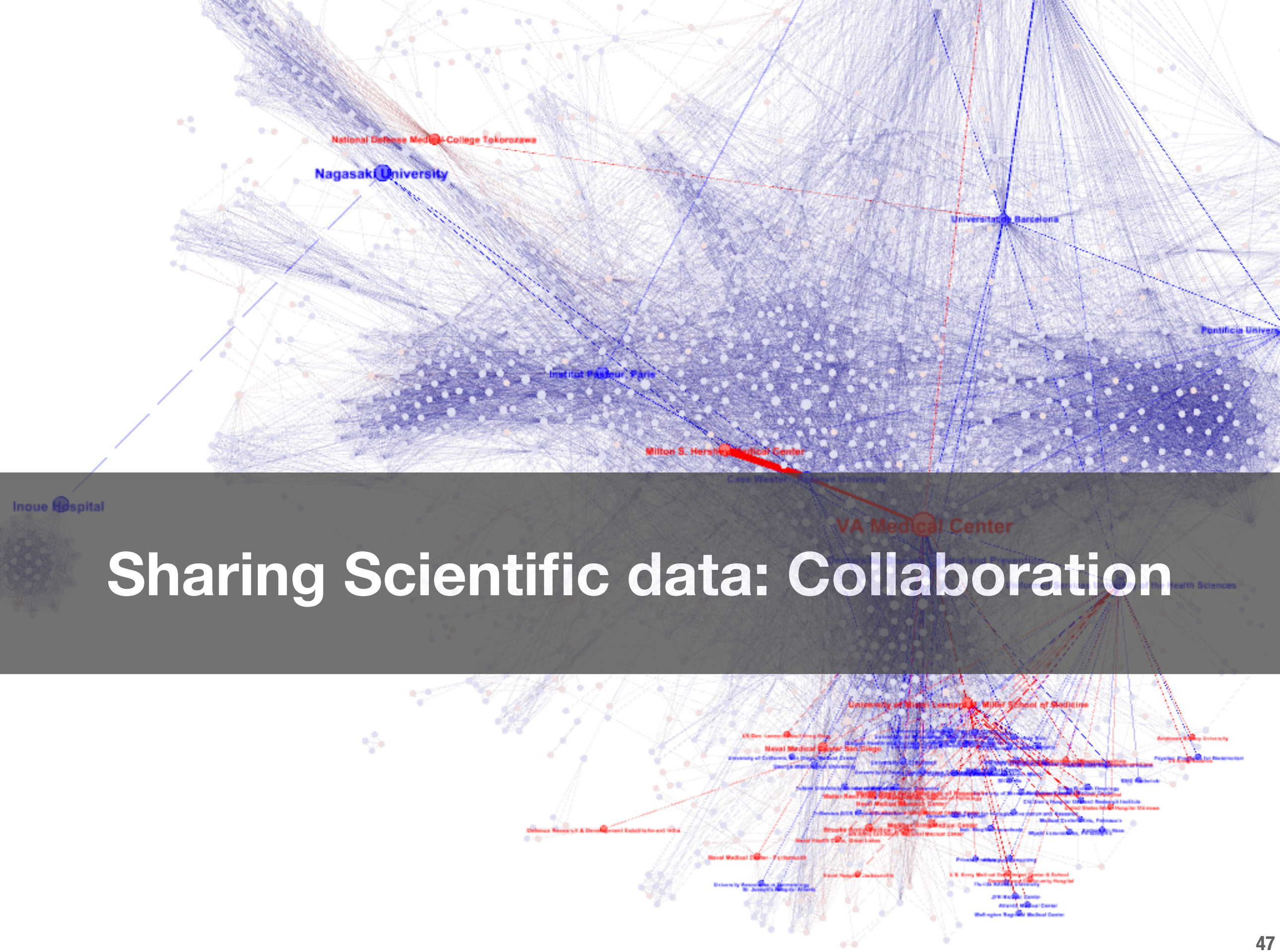
# Analyzing the data

# Compute == Answers!

The pinnacle of data transit, the reason we store it in the first place

- **High performance computing: clusters, supercomputers, single servers, powerful workstations, etc.**
- **Mostly a datacenter issue**
- **Unless…**
  - Storage not centralized or co-located: data duplicated unless have a killer network
  - New methods: data doesn't move, compute moves to data

# Sharing Scientific data: Collaboration



# Collaboration

## Fundamental to science

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- **Now that data production is reaching petascale, collaboration is getting harder**
- **Clinical collaboration is already difficult enough, increased data production in HIPAA environments, larger cohorts, multi-site studies**
- **Projects are getting more complex, more data is being generated, takes more people to work on the science**
- **Journal authorships: common to see 40+ authors now**
- **Clearly a networking problem at its core**
- **Let's face it, doing this right is *expensive!***

# Data Movement & Data Sharing

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The gist of collaborative data sharing in life sciences

- **Peta-scale data movement needs**
  - Within an organization
  - To/from collaborators
  - To/from suppliers
  - To/from public data repos
- **Peta-scale data sharing needs**
  - Collaborators and partners may be all over the world

# Network: ‘ScienceDMZ’

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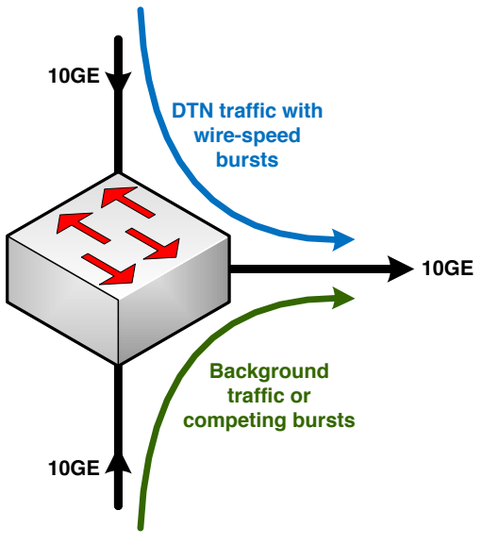
- **Very fast “low-friction” network links and paths with security policy and enforcement specific to scientific workflows**
- **“ScienceDMZ” concept is real and necessary**
- **Central premise:**
  - Legacy firewall, network and security methods architected for “many small data flows” use cases
  - **Not built to handle smaller #s of massive data flows**
  - Also very hard to deploy ‘traditional’ security gear on 10Gigabit and faster networks
- **More details, background & documents at http://fasterdata.es.net/science-dmz/**



# Simple Science DMZ:

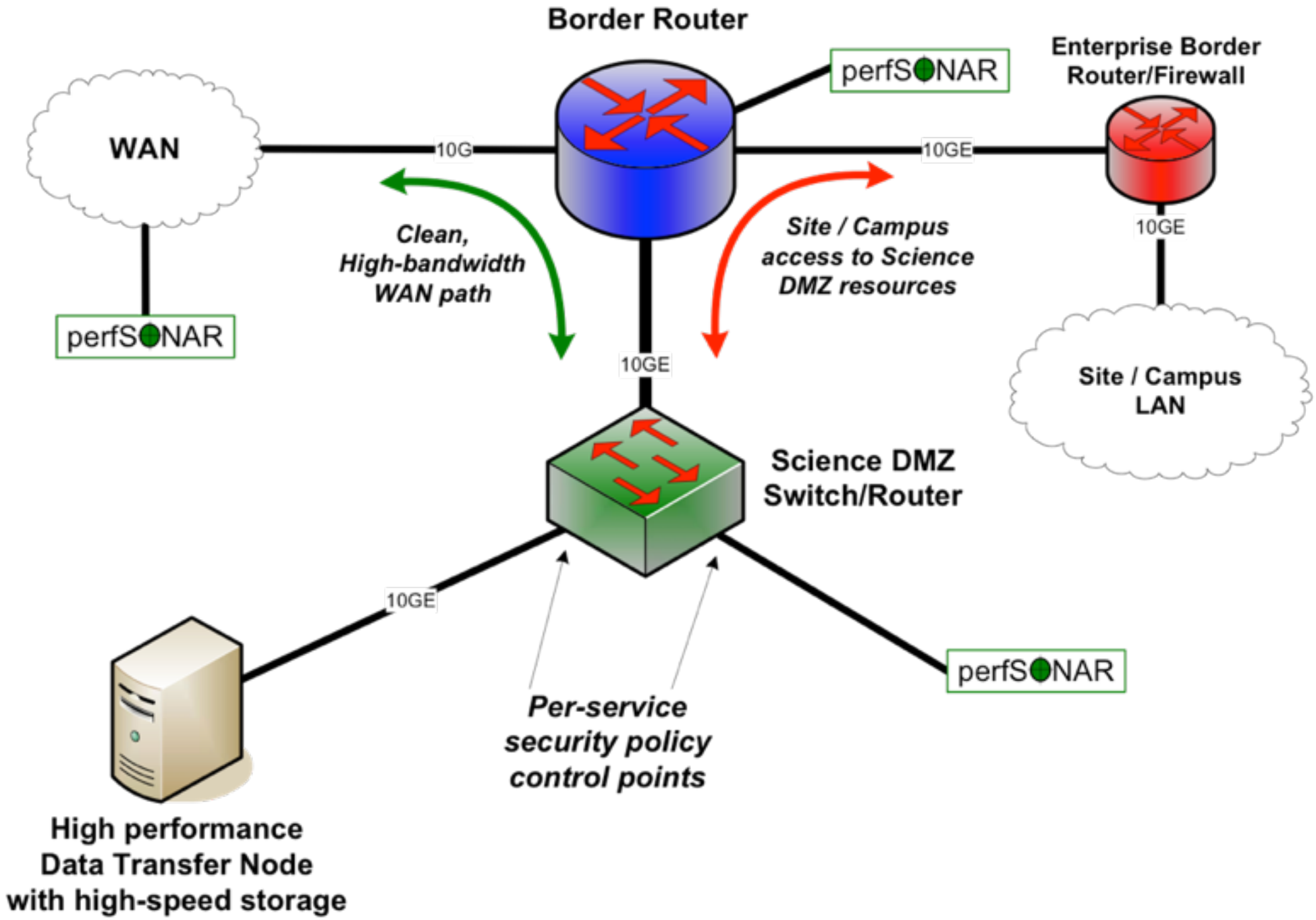



Image source: "*The Science DMZ: Introduction & Architecture*" -- esnet

# Standard Science DMZ

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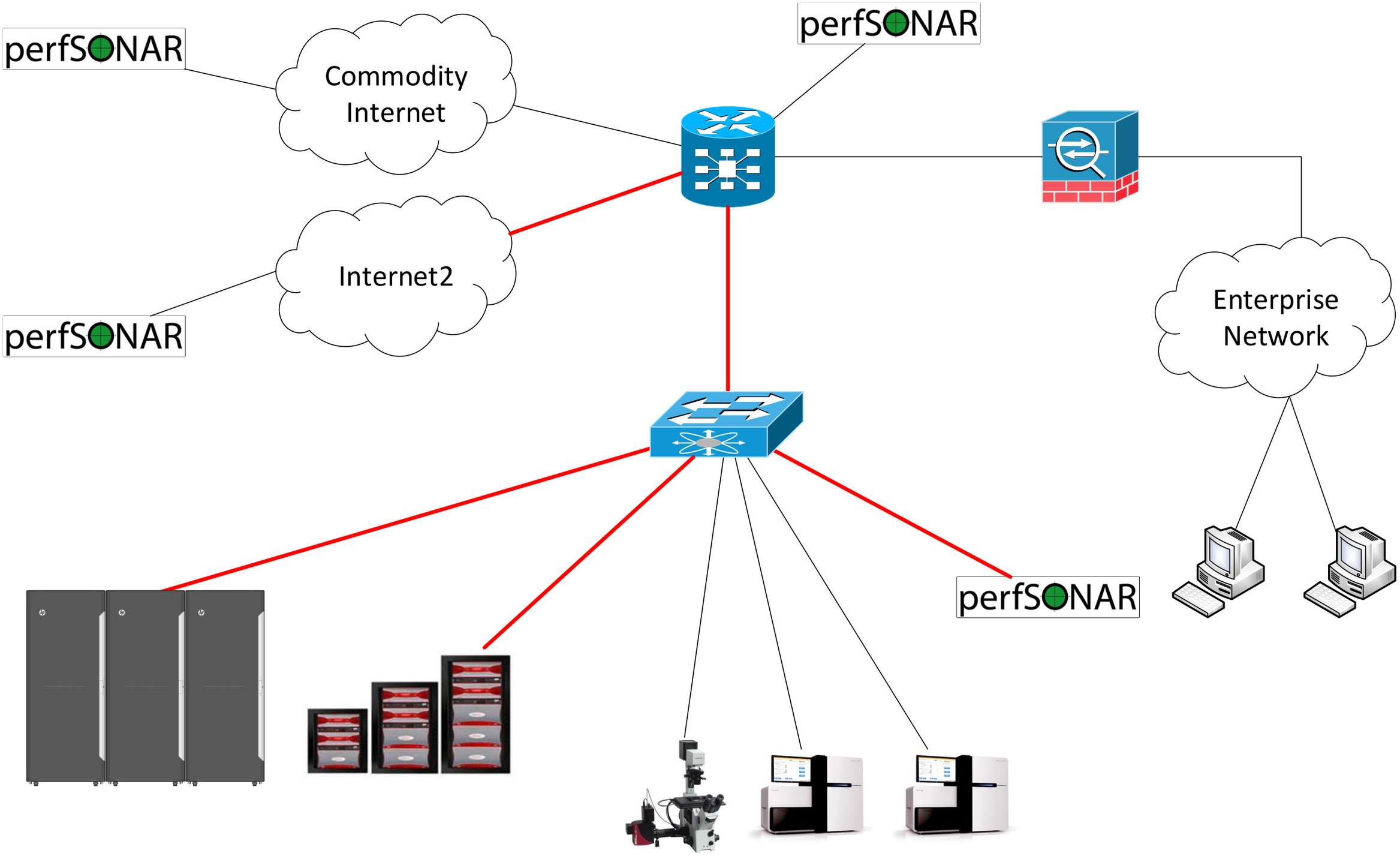

# Trusted/Untrusted Science DMZ

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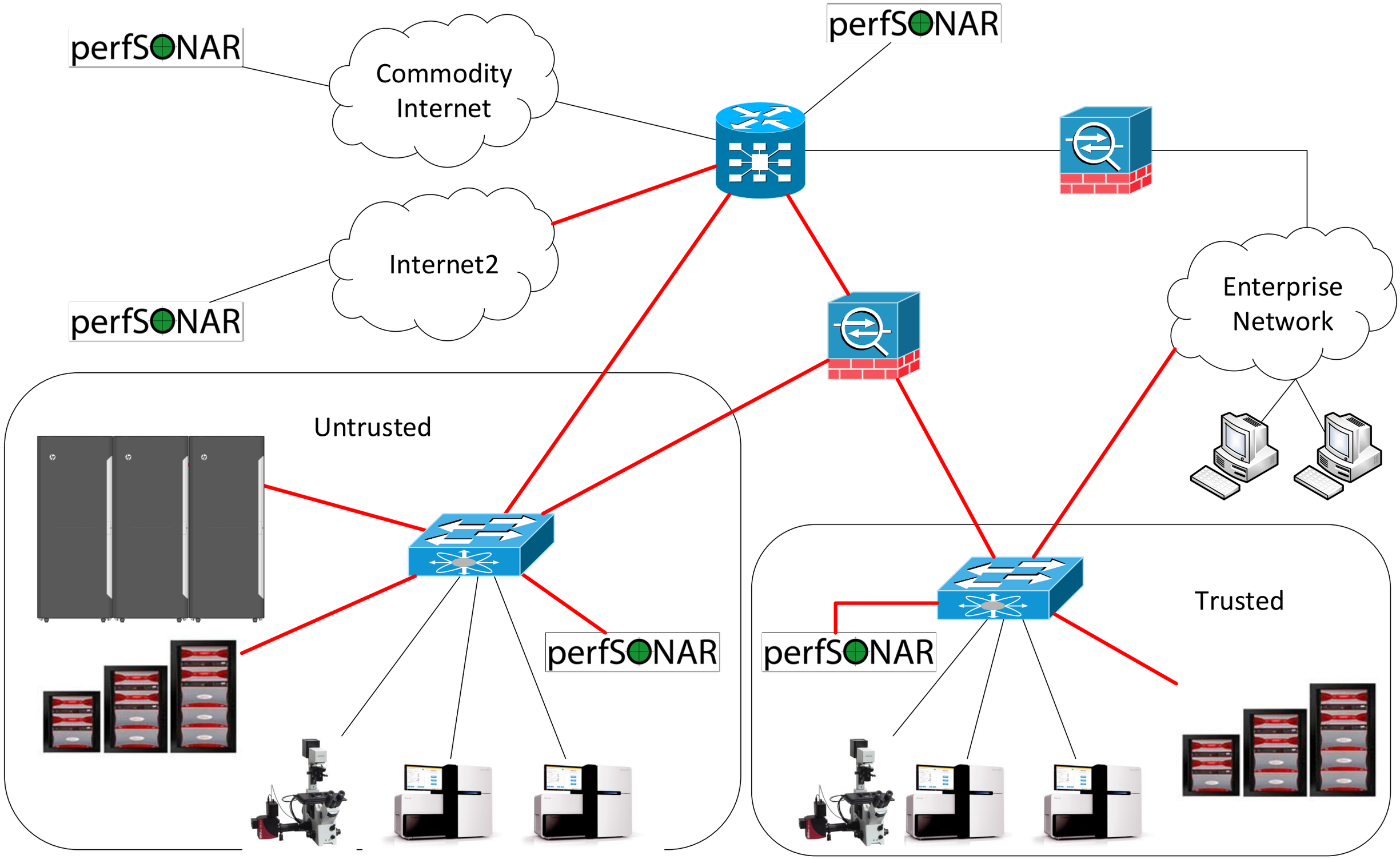

# Medical/Regulated Science DMZ

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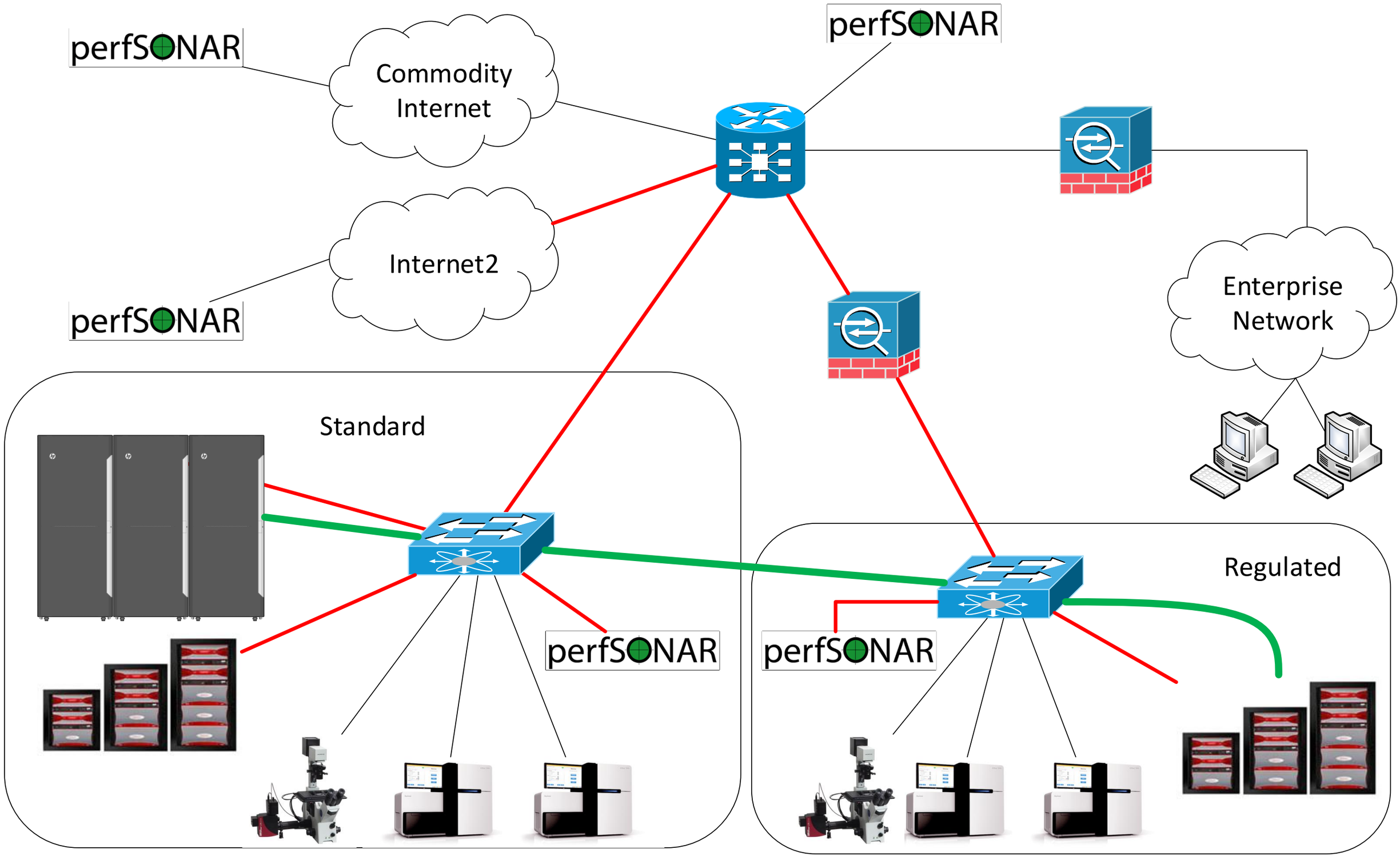

# Multi-site Science DMZ

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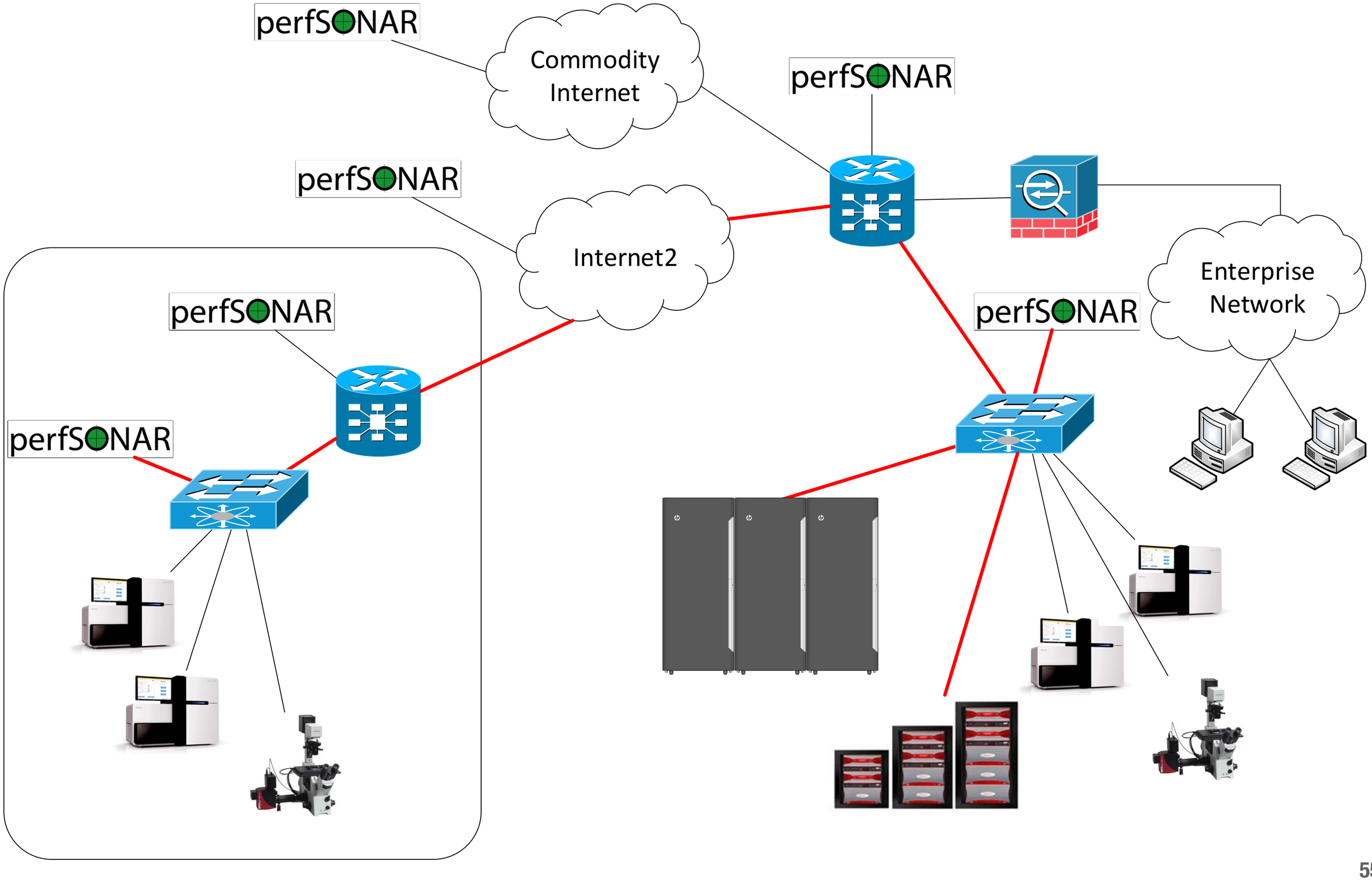

# What’s the Big Picture?

# [Hyper-]convergence

Make IT Infrastructure a research tool

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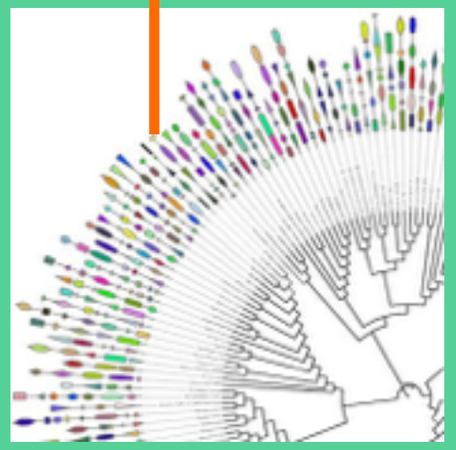
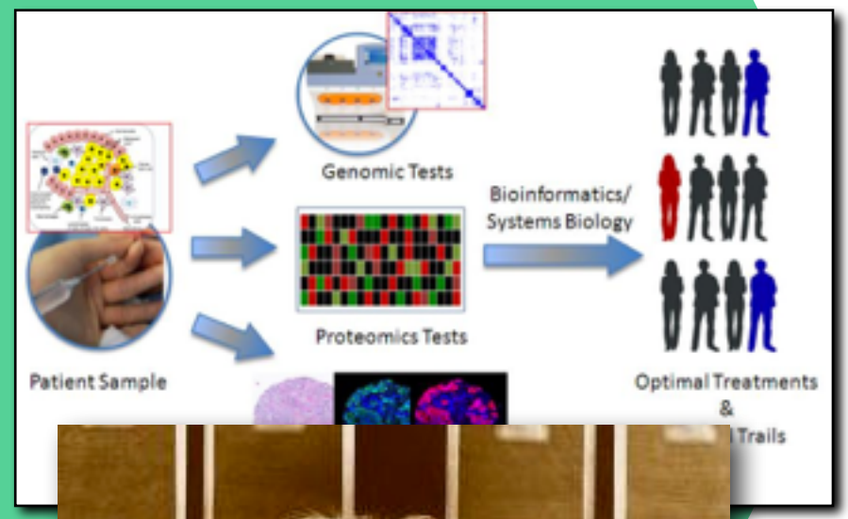
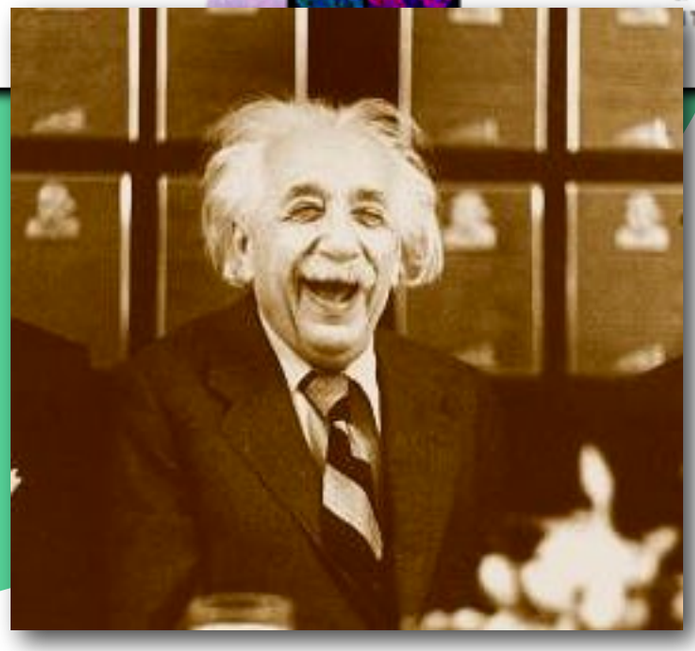
## Laboratory

## Converged Solution



## Knowledge



# Universal Truth

"The network IS the computer" - *John Gage, Sun Microsystems*

- **Convergence is not possible without networking**
- **Also not possible without GOOD networking**
- **Life Sciences is learning lessons learned by physics and astronomy 5-10 years ago**
- **Biggest problem is Org acceptance and investment in personnel and equipment**
- **Next-Gen biomedical research advancing too quickly: must invest now**

end; Thanks!