



# NSDF Development at CHESS

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NSDF All-Hands Meeting  
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# Cornell Laboratory for Accelerator-based ScienceS and Education

## CLASSE

- CHESS X-Ray user facility
  - Seven beam lines
  - Three sub-facilities, supported by the NSF, NIH, and AFRL
  - Macromolecular crystallography, structural biology, chemistry, quantum materials, and material science
  - New Experimental Hall to house the 20 Tesla High Magnetic Field beamline
- Accelerator Physics
  - CESR, CesrTA, SRF, ERL
- Particle Physics and Astrophysics
  - CMS, Cosmology, Muon g-2, HEP Theory, Theoretical Astrophysics
- Center for Bright Beams

<https://www.chess.cornell.edu>

<https://www.classe.cornell.edu/Research/>

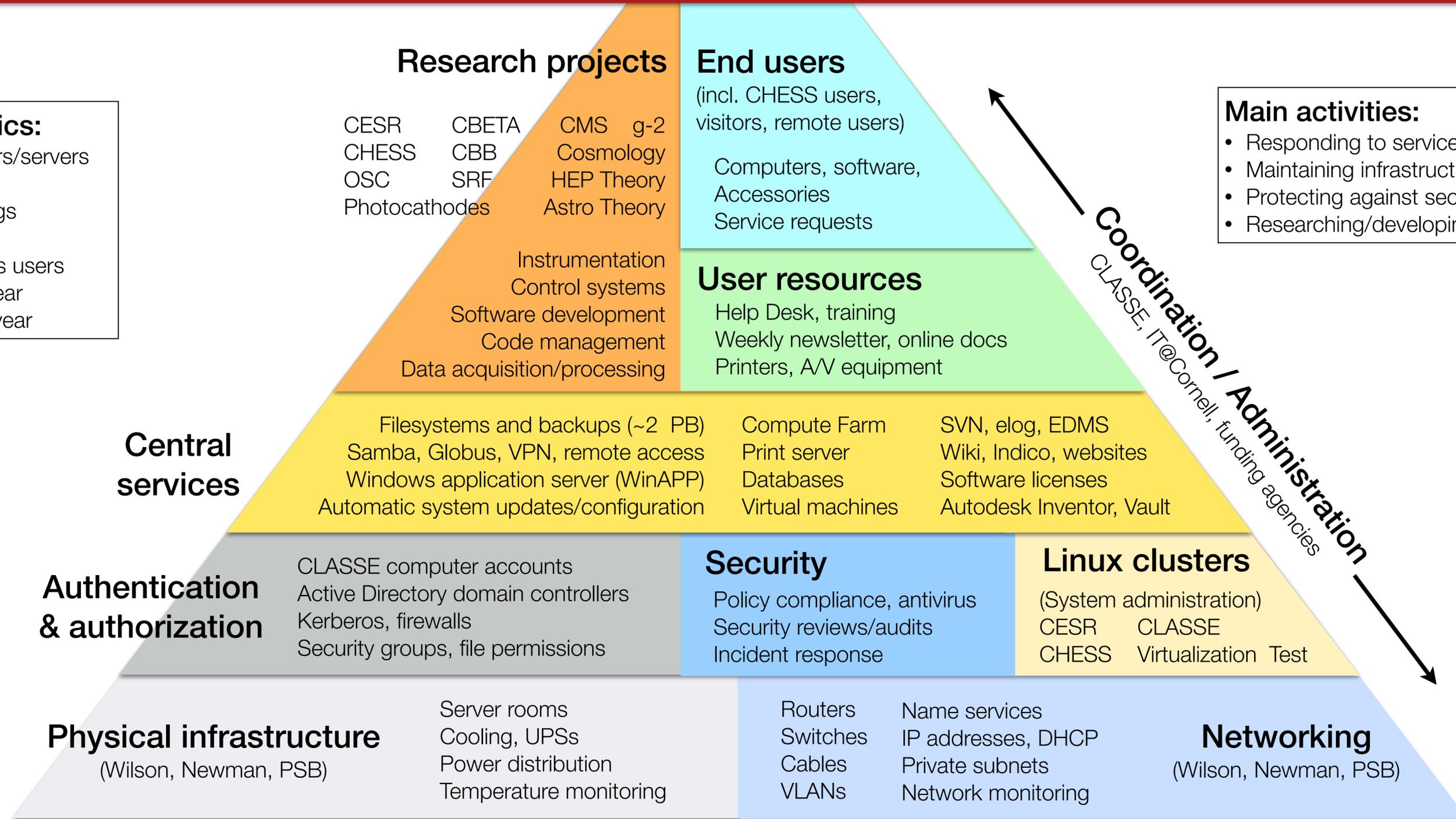




# CLASSE Cyberinfrastructure

## Some statistics:

- 500+ computers/servers
- 3 major OSs
- 3 major buildings
- 60+ networks
- 250 on-campus users
- 1000 visitors/year
- 3000+ tickets/year



- ### Main activities:
- Responding to service requests
  - Maintaining infrastructure and services
  - Protecting against security threats
  - Researching/developing new capabilities



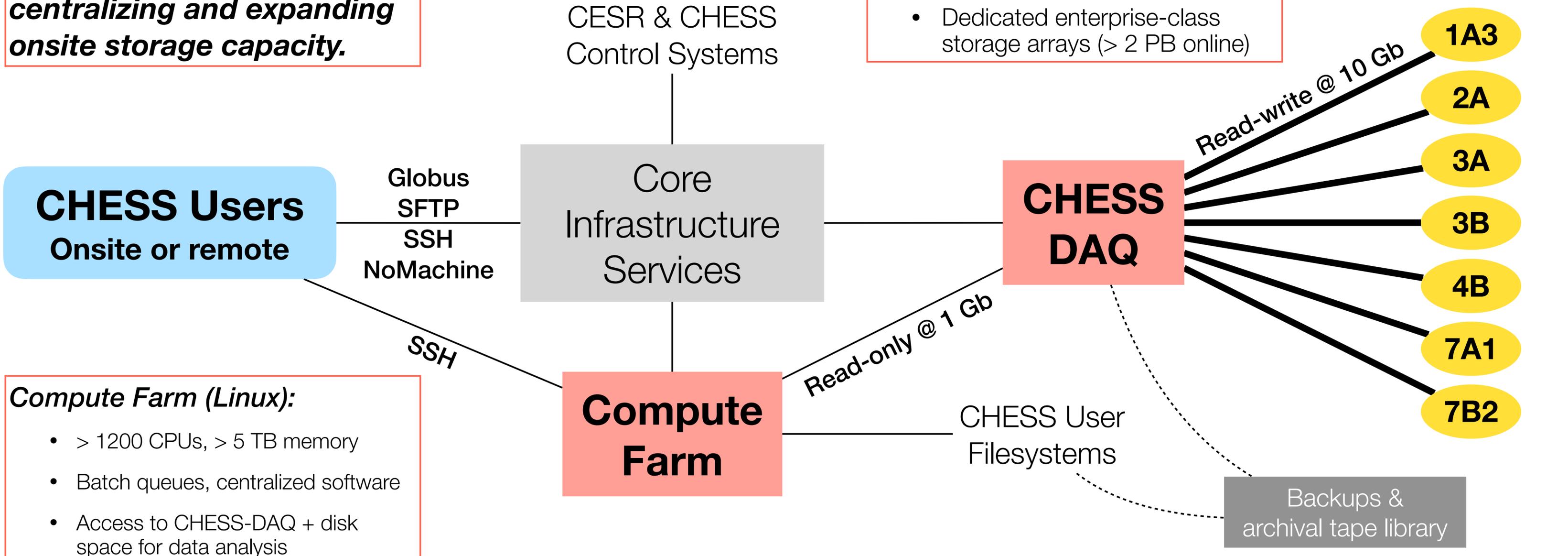
# CHESSE Cyberinfrastructure

**Over the past few years, CHESSE has addressed growing data volumes by centralizing and expanding onsite storage capacity.**

## CHESSE-DAQ:

- High-speed 10 Gbps fiber data collection network
- Dedicated enterprise-class storage arrays (> 2 PB online)

CHESSE Experimental Stations



**Compute Farm (Linux):**

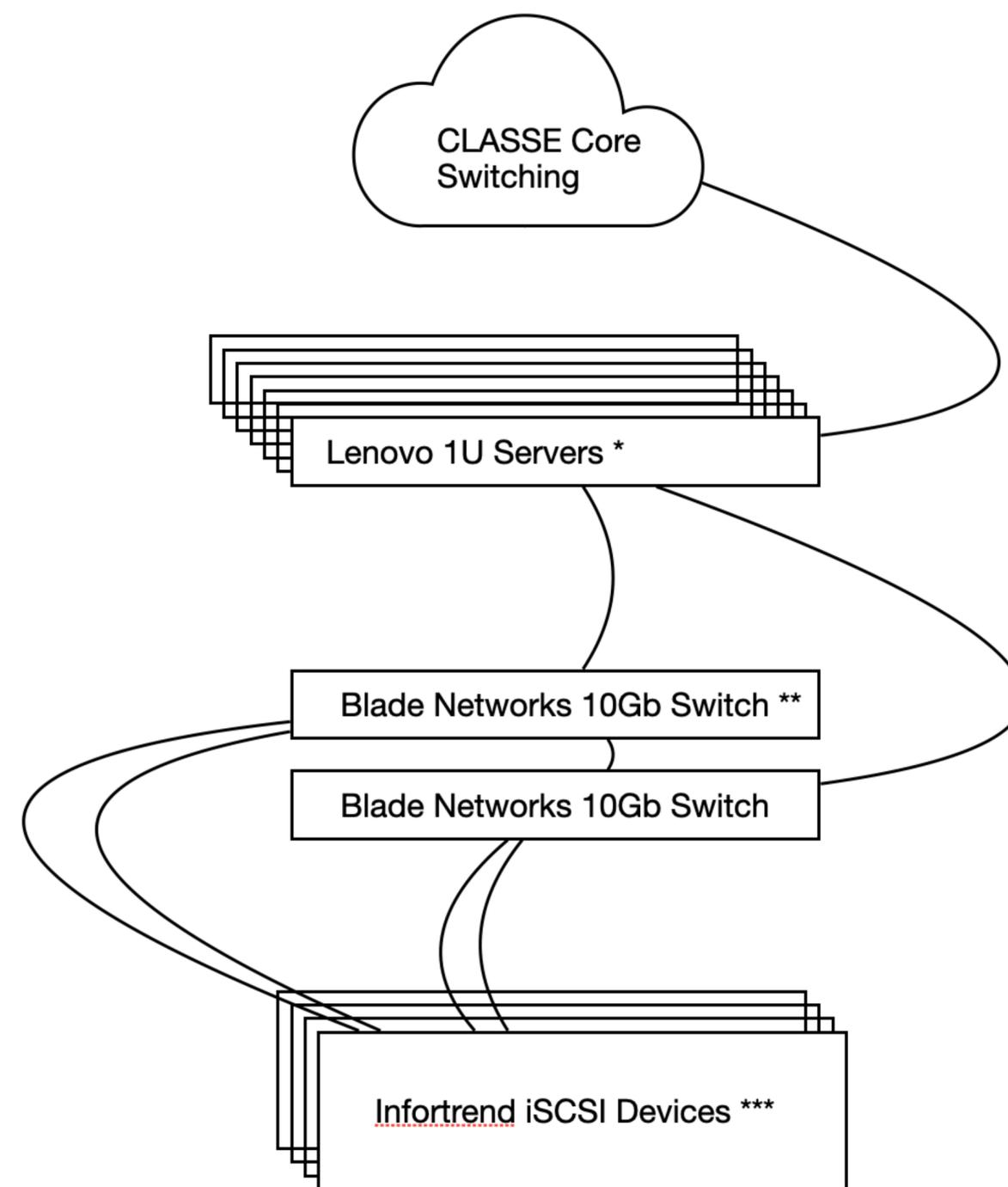
- > 1200 CPUs, > 5 TB memory
- Batch queues, centralized software
- Access to CHESSE-DAQ + disk space for data analysis



# CHESS Cyberinfrastructure

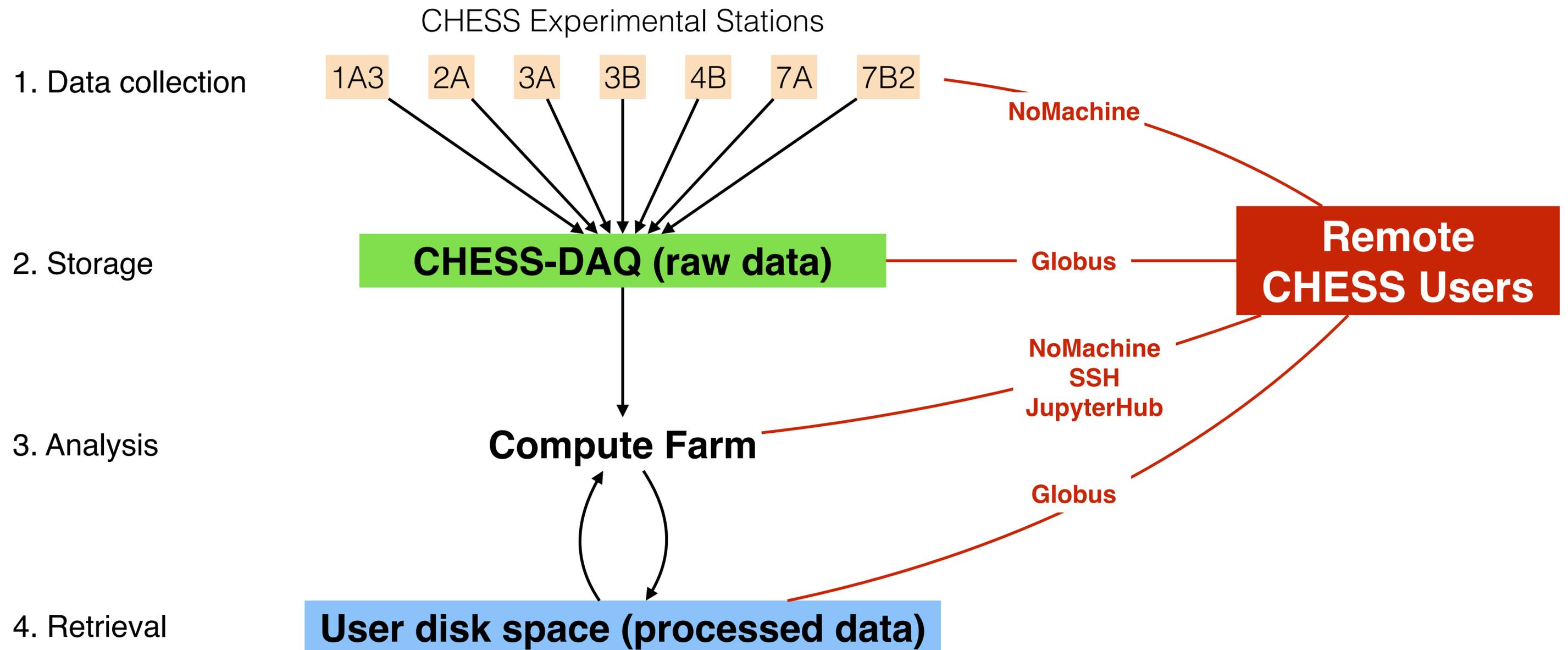
## High-performance computing at CHESS:

- Core infrastructure and experimental control systems: Linux high-availability clusters
- Dedicated private networks, highly segmented for performance, security, and personal and equipment protection
- Station computers and dedicated GPU and CPU analysis nodes, supporting in-line analysis, reduction, and processing
- GridEngine queuing system supporting batch, GPU, interactive, and parallel jobs.
- Managed end-user computers (Windows, Linux, Mac) for data collection, hardware control, and personal productivity





# CHES User Workflow





# CHESSE Operations

## **Three run cycles per year, on average providing 125 days of beam time to users.**

- 24/7 user operations during run, typically one user group per beam line per week.
- Users can apply for beamtime each cycle through general user proposals and beamtime requests (BTRs) in the web-based user portal.
- On average ~150TB of raw data collected each run

## **Three extended downs each year**

- Maintenance and upgrades.
- Machine Studies.
- Archival and rotation of raw data from previous run.
  - 2023-1 archived to tape
  - 2022-3 removed from disk
  - Directories initialized for 2023-2
- Alignment.



# NSDF Development at CHESS

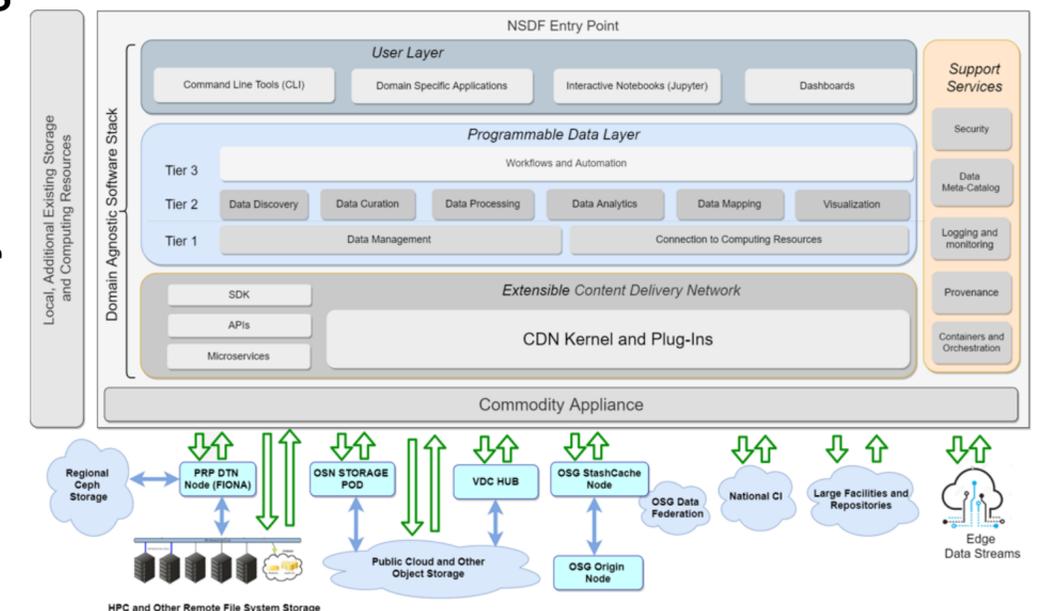
## Initial exploration and development

- CLASSE accounts created for developers and collaborators, with access to a login node for initial development.
- Initial deployments using docker and singularity.
- Data accessed locally over NFS, and transferred between sites using Globus.

## NSDF Entry Point - [nsdf01.classe.cornell.edu](https://nsdf01.classe.cornell.edu)

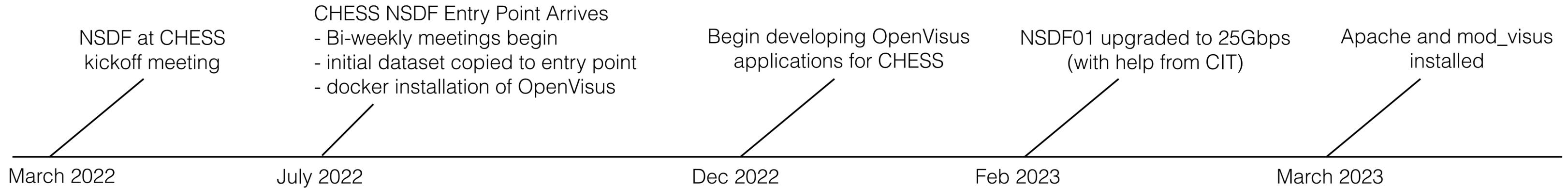
- Standard CLASSE Scientific Linux 7 OS install
- 131TB RAID6 (with one hot spare) using mdadm, from twelve 16TB drives
  - XFS filesystem mounted at /mnt/data1/, exported internally at /nfs/chess/nsdf01/
  - Data accessed locally over NFS, and transferred between sites using Globus
- Two INTEL XEON GOLD 6252N 2.3GHZ processors
- 512MB PC4-23400 2933MHz memory
- One Broadcom P425G 25GbE 4xSFP28 PCI4 card
  - 10Gb connection to CLASSE Public subnet - [nsdf01.classe.cornell.edu](https://nsdf01.classe.cornell.edu)
  - Accessible through firewall via https, ssh, sftp, and scp

NSDF Entry Point





# Software and Service Installation

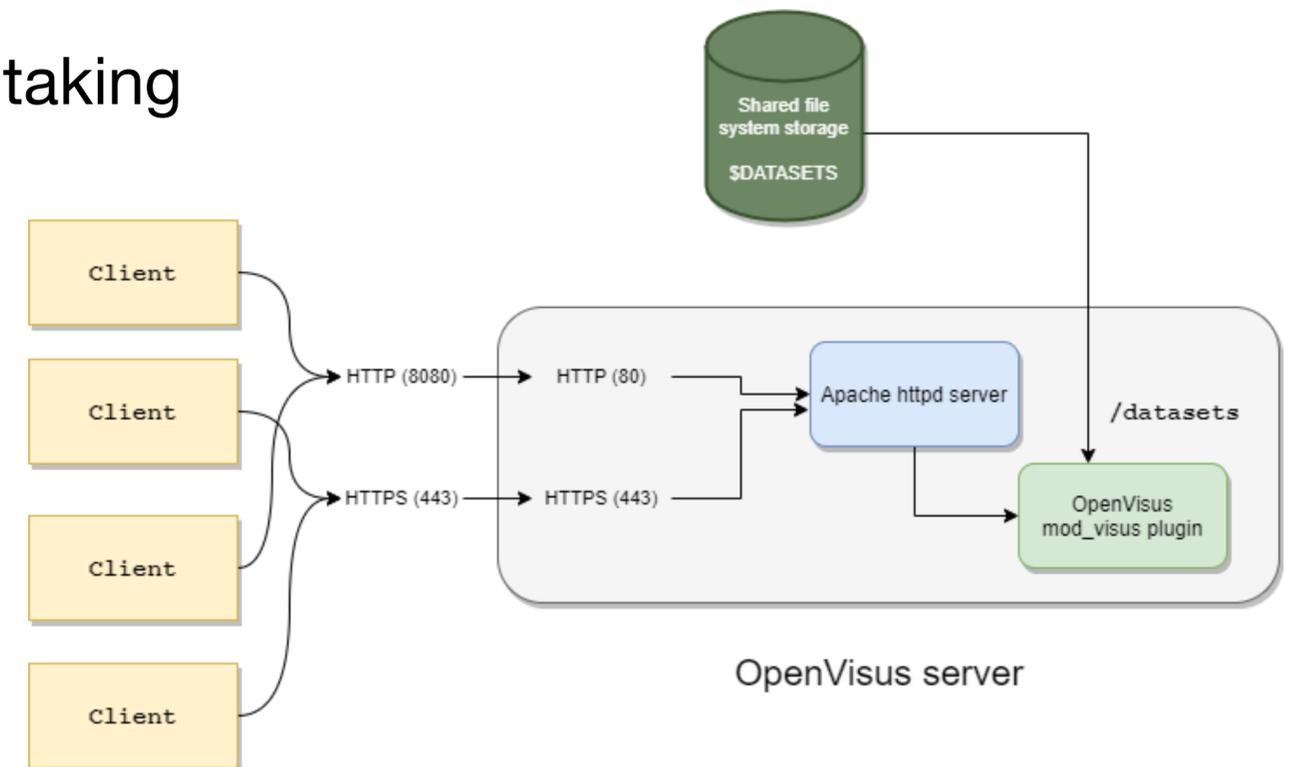


## OpenVisus installation

- nsdf security group for managing docker containers
- nsdf service account for managing centralized installations and configurations, and for running production services
- Developing visualizations to be used in real time during data taking

## Apache mod\_visus deployment

- Server installation of OpenVisus
- sudo privileges granted to nsdf security group for updating configuration, restarting apache, and viewing log files
- Apache basic password authentication.





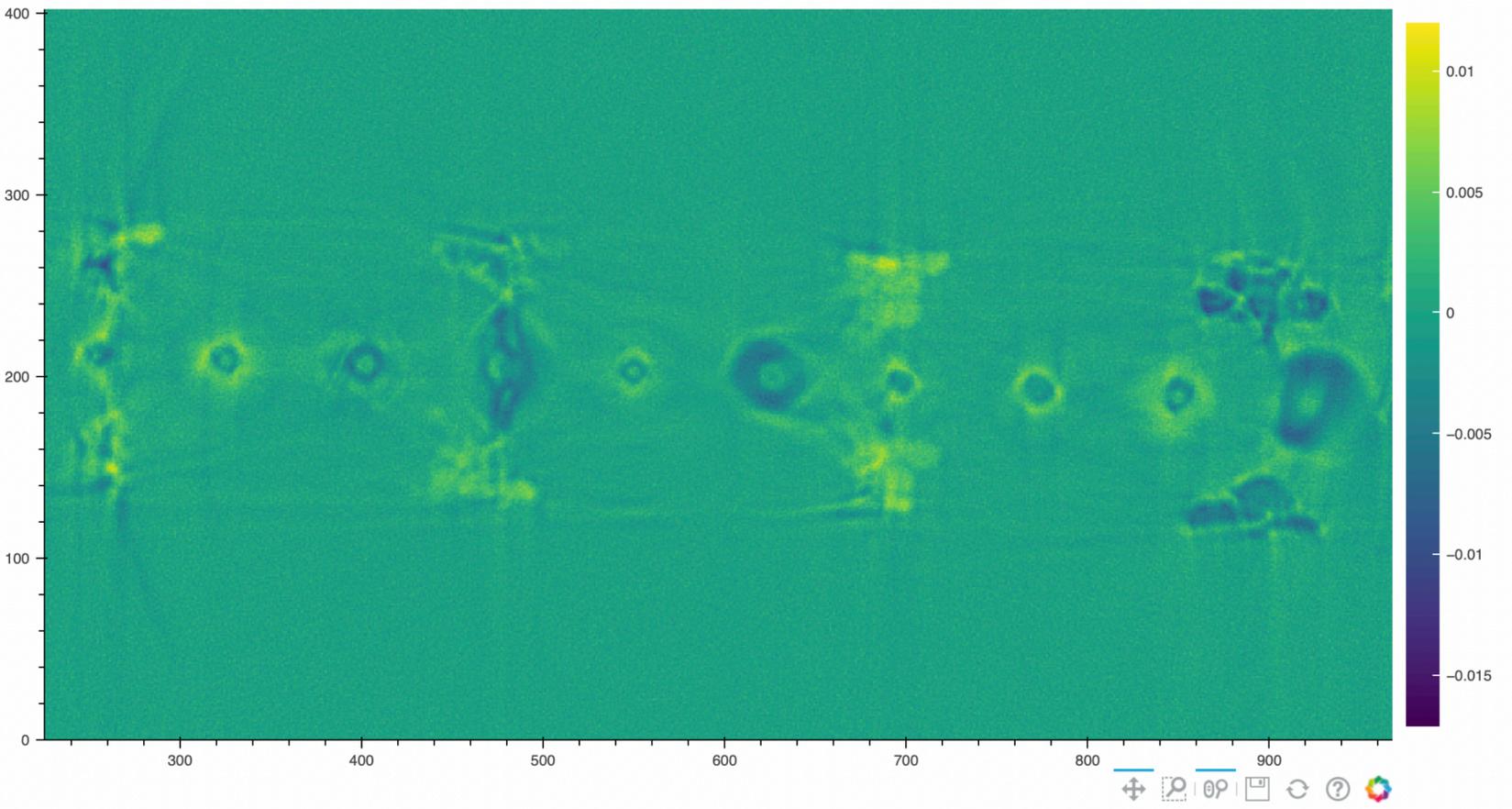
# Visualizing CHES data with OpenVisus on the Entry Point

```
def MyApp(doc):
    db=ov.LoadDataset(idx_filename)
    slices=Slices(doc,sizing_mode='stretch_width')
    slices.setPalette(palette, palette_range=(m,M))
    slices.setTimeStep(db.getTime())
    slices.setField(db.getField().name)
    doc.add_root(slices.layout)
    doc.add_timeout_callback(lambda: slices.setDataset(db),100)

ShowApp(MyApp)
```

jupyter01.classe.cornell.edu  
<https://jupyter01.classe.cornell.edu/user/wms8/proxy/37187>

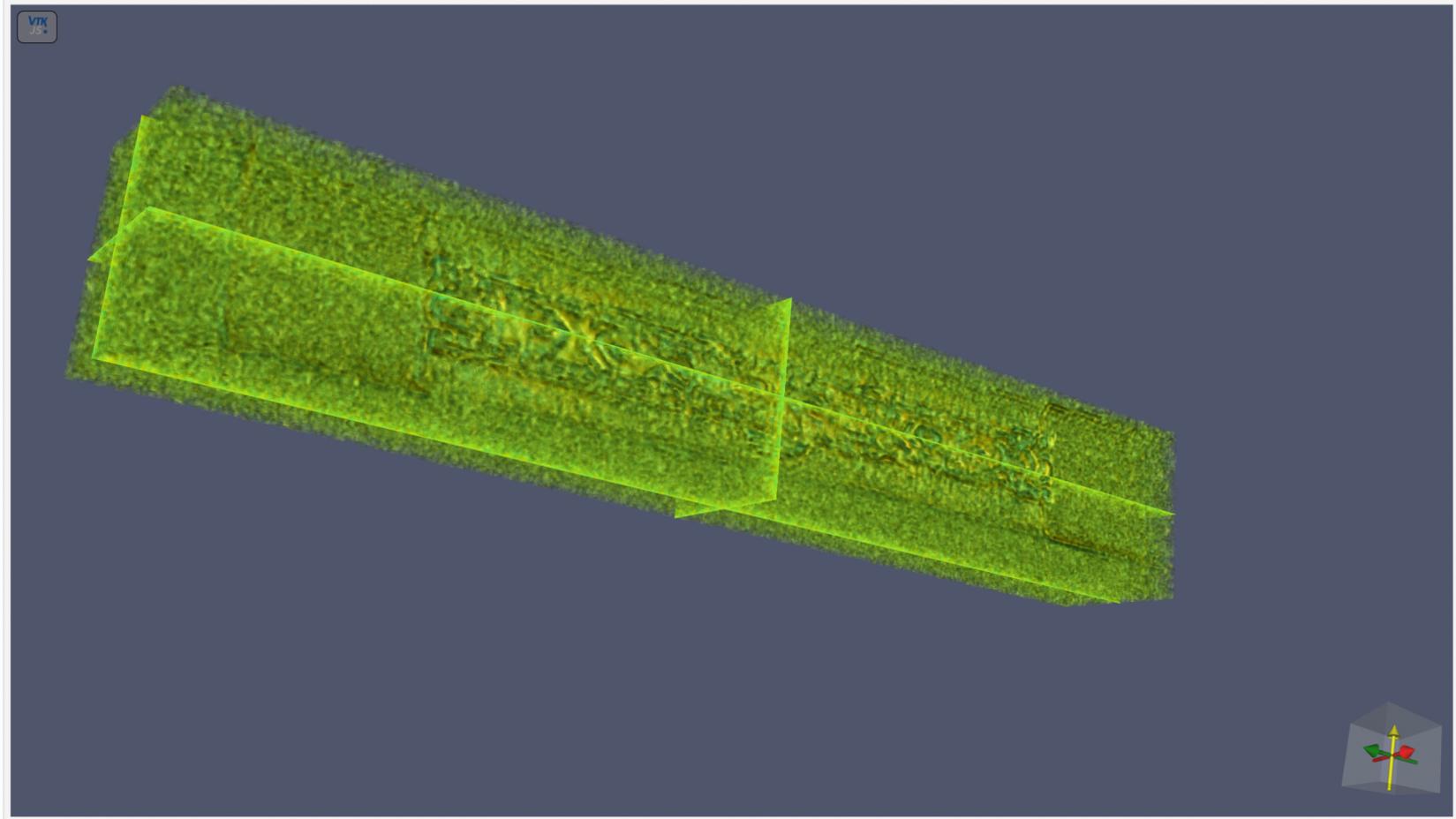
Layout Palette  
 3 Viridis256  
 Direction Z Offset: 165



```
css_classes=['panel-widget-box'],
sizing_mode='stretch_width',
width_policy='max')
```

Scalar fields names= ['data']  
 Dataset [x,y,z] dimensions= [1193, 402, 330]  
 db.read returned shape (42, 51, 299) dtype float32

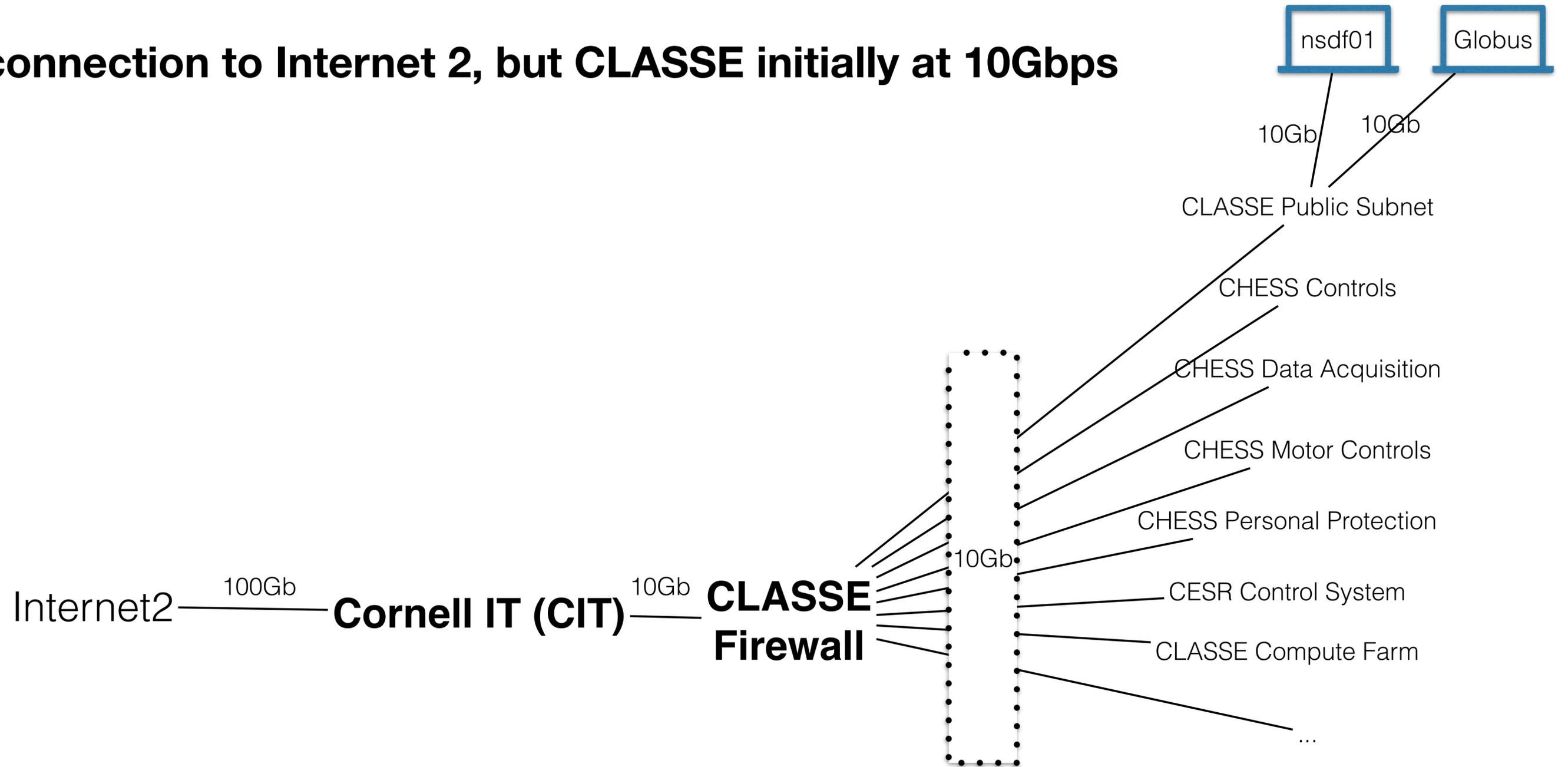
Experiment: 2  
 i-slice: 21  
 j-slice: 25  
 k-slice: 149  
 Show Volume  Show Slices





# CHESS Network Layout

**CIT has 100Gb connection to Internet 2, but CLASSE initially at 10Gbps**

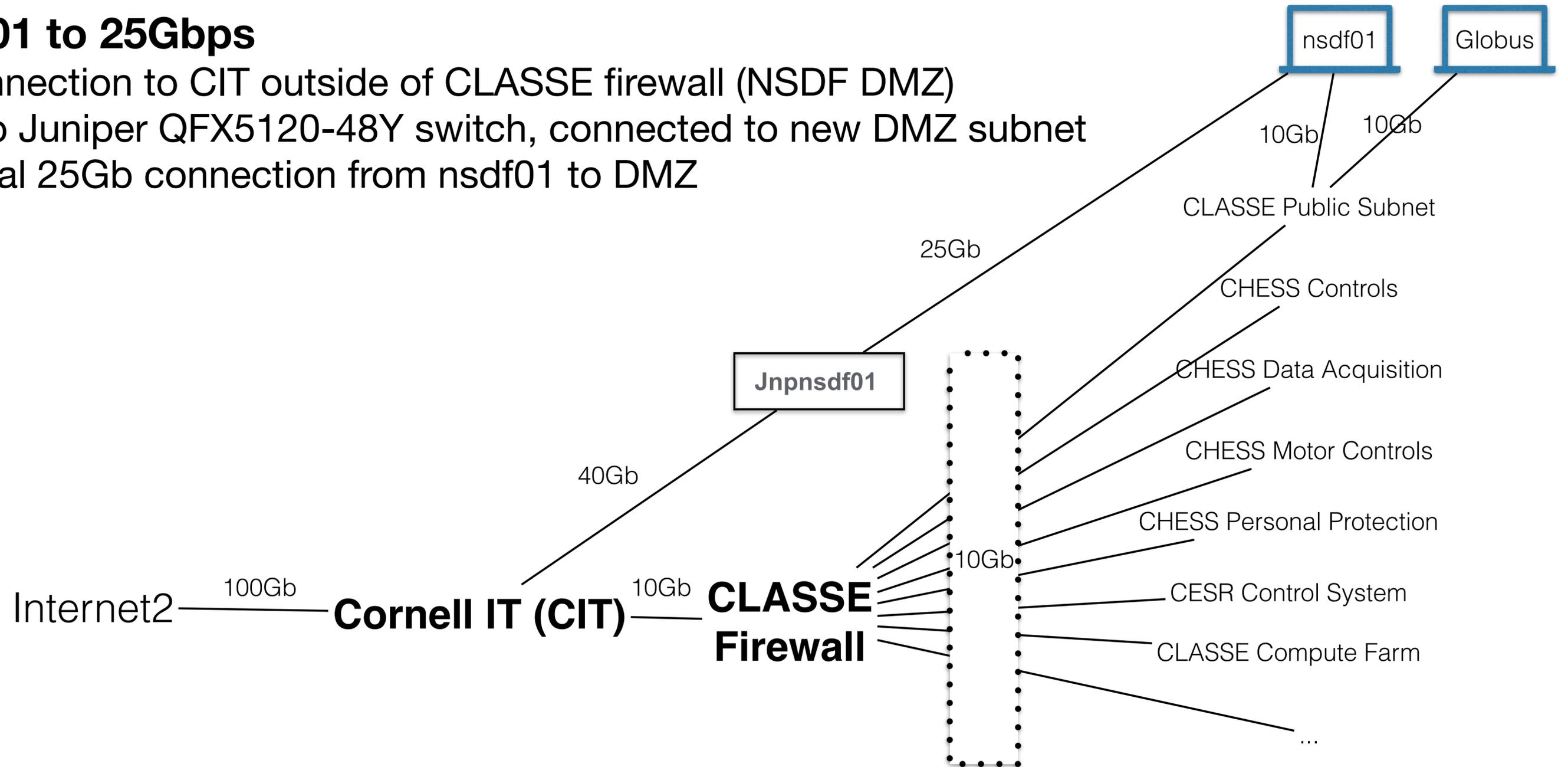




# Network Upgrades

## Upgrading nsdf01 to 25Gbps

- New 40Gb connection to CIT outside of CLASSE firewall (NSDF DMZ)
- Procure 100Gb Juniper QFX5120-48Y switch, connected to new DMZ subnet
- Install additional 25Gb connection from nsdf01 to DMZ





# Future Developments

## Cyberinfrastructure Upgrades

- Upgrade nsdf01 entry point to 100Gb connection to Internet2
- Upgrade internal backbone to 25Gb or above
- Migrate to Ceph storage cluster
- Upgrading to Alma 9
- Kubernetes

## Data Visualization

- Gathering requirements from scientists in efforts to develop OpenVisus based visualization to be used in real time during data taking by remote experimenters.

## NSDF part of concerted scientific computing efforts initiated in 2021

- Workflows/services, metadata management, large-scale code design, statistical models/algorithms, AI/ML, HPC/HTC
- Exponential growth in data volume
- Complexity of user experiments and analysis software



# Thank You

**<https://www.chess.cornell.edu>**

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