

Information Technology Division^{**}

High Performance Computing Center



Perspectives in Storage **Considerations for Academic and Research Computing**

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Lustre User Group Meeting — Texas Tech University, Lubbock, Texas — May 8, 2024

Four Basic Considerations for Academic Computing

and research computing, data handling, and service delivery:

- 1) How do they serve the *core functions* of the university or institution?
- 2) What is the *return on investment* in terms of those core functions?
- 3) With what speed and performance can needed services can be delivered?
- 4) What *provenance and protections* need to be applied to the services?

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Four basic questions need to be answered for delivery of support for academic

To answer these questions in terms of how they apply to storage, let's examine them one by one, then project some recent and emerging trends to the future.







Core Functions

Some organizations still consider academic computing and data resources to be *cost centers*.

A better perspective for academic and research computing services is that in most cases, they are more accurately represented in financial terms as *profit and productivity centers*, and that they play an essential role in non-financial academic and research productivity that are best viewed in terms of their support for the *core functions* of the institution.

Research grant income	Academic Productivity	Publications		
Discovery potential	Courses taught	Community impact		
Student skills	Knowledge growth	Patents and IP		
Awards & recognition	Innovation	Outreach and Training		









Core Functions

is through its support for these core functions:

- How can data services including storage systems be deployed in ways that support the core activities of the institution?
- What data handling capabilities are needed, including backup, access, performance, security, indexing, metadata, long-term storage, archival, retrieval, disaster recovery, summarization, data mining (including AI), etc.?
- How can these be achieved within the resources available to the organization?
- Which of these are formal mandates from funding agencies, government, or the institution and which are optional?

The best way to view the role of storage in academic and research computing







Core Functions

One problem among many is that considerations with respect to data often come in the form of **unfunded mandates**: the institution is requested or expected to take care of issues with respect to data without explicit or identified funding sources to handle these requirements.

This situation is only going to get **worse** in the near future. Government mandates for data protection are increasingly becoming part of the conditions for receipt of grant funding, and individual faculty members or research groups usually don't have, and do not budget for, the systems needed to put such protections into place.

In terms of academic computing more broadly, **increasing use of data** by pretty much every field of study is a trend that has been growing for years, and has been catapulted into very visible view by the emergence of **large language models**, **machine learning**, **and other Al-related methods** now making their way into essentially all academic work.

By and large academic organizations are not prepared to handle this onslaught of data!



Return on Investment

A poorly understood, often mentioned, but difficult to define aspect of academic and research computing and data services support is the topic of **return on investment**: what does the organization get back or provide to its constituents from the various investments that it makes in providing these services?

Although this may seem at first far from the technical details of storage systems, it is **essential** in my opinion to understand the context of such systems in these terms in order to see where they fit into academic computing in general and in order to determine what services are needed, as well as to make **informed choices** about what type and quantity of services are needed.

There are several challenges in this area, but it is possible to approach them systematically. In fact, a summary of the rest if this talk is that it is *necessary* to approach them systematically to have any hope of being able to make sense of the multiple demands being presented in the context of data services and storage.



Definition of "Return"

Simplest form: Financial aspects

- Raw value of externally funded research supported
- F&A / indirect costs obtained through such research
- Charges to users for access to research computing and data infrastructure
- Cost avoidance compared to other methods of resource or service delivery

This is an easy set of statistics for you to gather for each method of delivery!

aggregate on any level, and even fewer reported these to upper administration.

While simple to define, this metric varies depending on aspects you want to measure:

- Despite this simplicity, relatively few institutions in our survey gathered such statistics in



Examples of Financial ROI factors

Stewart et al., PEARC19, https://doi.org/10.1145/3332186.3332228

Area of Benefit	Measure of Benefit	Ways to Measure Benefit		
Grant income	Monetary income from grants and F&A	Measure income attributable to use of the resources		
Products & patents	Monetary income from licenses and spinoffs	Allocate part of income attributable to use of resources		
Economic impact	Regional economic impact as measured by economic models (IMPLAN)	Indirect financial benefits, jobs, & tax income attributable to existence of resources		
Productivity of end users of CI facilities in research	Financial value of time saved	Cost of the time that would have been spent by end user doing research without use of CI resources		
Cost avoidance for Cl resource delivery	Value of investment in other CI facilities that would have been made without use of a particular facility	Actual costs, cost avoidance		
Cost avoidance though personnel resources	Value of support and consulting from CI resource provider	Evaluate allocated usage as a fraction of total costs for providing support and consulting		
Training value	Value of training materials created by organizations operating CI facilities & knowledge gained by users	Perceived value, equivalent cost of commercial training, value of CI skills held by employee entering job market		





Definition of "Return"

Non-financial aspects

Most organizations place definite value on factors other than dollars received:

- Publications and academic output
- Training and instruction to students, staff, & faculty
- Recruitment and retention of forefront researchers
- Familiarity with computational and data science research methods
- Speed to research output

Important aspects of return *must be defined in the context of your organization*



Examples of Non-financial ROI

Stewart et al., PEARC19, <u>https://doi.org/10.1145/3355738.3355749</u>

Table 2					
Output	Outcome	Nonfinancial measures of outcome	Impact		
New discoveries reported in publications	Publications	Number of publications, citations of publications, impact factors of publications (and the journals in which publications appear	Improved quality of life for people		
Productivity	Shorter time to publications	Time saved	Better management of natural and personnel resources		
People trained in areas in which they would otherwise not have been trained	A better-trained STEM workforce	Increased salary, greater employment security for the individual	A better-trained workforce for the economy; Improved global competitiveness for any given country		
Awards, press notices	Any award, e.g., Nobel Prize	Numbers, types of awards	Recognition of a particular invention's significance; reputational benefits for the people and organizations winning the award		
Patents and licenses	An invention is legally protected by exclusive use of the patent holder or licensee	Number of patents	The invention may become a commercial product, or may be used in commercial products that improve people's quality of life, and the sustainability of human life on Earth		

Table C





Definition of "Investment"

Organizational factors

far beyond the raw cost of purchasing just equipment or cloud contracts

- Creating conditions for faculty, researchers, and students to be productive
- Providing adequately robust, backed-up locations for data storage
- Investing in personnel training to provide support staff
- Promoting and encouraging use of modern, efficient, up-to-date methods
- Providing self-help methods to allow and encourage learning and development
- Making use of national and international resources beyond your institution

The exact nature of *investment* on the part of the institution may and usually does extend





Definition of "Investment"

Monetary - hardware, operations costs, and personnel

To understand a given institution's investment in providing access to academic and research computing and data resources requires a *comprehensive view:*

- Differential cost to provide physical space, equipment, and other hardware capital investments
- Electrical power, cooling, and maintenance for on-premises equipment
- Contracting costs for externally provided cycles and storage
- Administrative expenses, including procurement and contract management
- Personnel costs for professional staff including consulting and support



Examples of investment factors

Monetary - hardware, operations costs, and personnel

Area of Expense	Purpose of Expense	Ways to Measure Investment		
Hardware acquisition	Computational and/or storage resources	Cost to purchase amortized over useful lifetime		
External/cloud resources	Computational and/or storage resources	Annual cost of contract and any applicable overage		
Maintenance costs	Service contracts or repair and replacement of on- site equipment	Costs of contracts or unscheduled mainetnance		
Electricity and cooling	Direct power to on-site equipment including power needed to provide cooling	Cost of electricity used and facility cost for cooling		
Data ingress/egress fees	Most applicable to off-site (cloud) resources	Annual cost of contract and any applicable overage		
Machine room space	Provide physical location for on-site resources	Differential cost compared to use of that space for other institutional purposes		
Software	Software to run on either on-site or off-site resources, as well as to retrieve and analyze results	Licensing costs, personnel support for either on-site or off-site usage, cost avoidance compared to other tools		
Training	Reduce time cost to researchers and/or support staff to use or provide access to resources	f Direct cost of externally contracted training, portion of staff time devoted to delivering or receiving training		





Comparing ROI for different approaches

If you don't measure ROI, you have no basis for comparison!

From previous research conducted and confirmed by the multi-year longitudinal CASC open community Cloud and Data Center Usage Survey summarized above, we see that there are many factors that enter into the definition of both the numerator (return) and denominator (investment) of the financial part of the ROI equation.

Non-financial aspects of both return and investment also need to be considered.

The exact relationship of factors for these comparisons varies greatly among institutions, and relative weights and importance assigned by the institutions will also vary.

Most institutions that undertake an effort to study ROI find strongly positive results for use of academic research computing and data resources, and a positive impact on their organizations and supported communities.*

* Chalker et al., PEARC20, https://doi.org/10.1145/3311790.3396642



Comparing ROI for different approaches

Related conclusions from CASC surveys and the above papers:

In addition to the above conclusions, here are some important survey results:

- Only a small fraction (25-30%) of institutions reported measuring or reporting ROI to their upper administration on a regular basis.
- Only a small fraction has yet explored cloud for large-scale usage.
- Large-scale institutions were more likely to have tested cloud for production but less likely to report cost savings for bulk computing tasks.
- Definite use cases exist for cloud usage, but these are so far mostly not driven by cost considerations.

The tradeoffs between the factors described here depend on the institution.



Return on Investment Summary

Here are the basic conclusions from the ideas presented so far:

- Factors entering into both the numerator and denominator for ROI vary by institution, and need to be considered across a broad range.
- So far, in three surveys, only a small fraction of institutions regularly gather and report ROI information internally or externally.
- Most institutions that do measure and report ROI for academic and research computing and data support find *a positive story to tell*.

proposal-based resources for your researchers and institution.

This same approach can be applied to storage services.

- A useful approach is to measure ROI including all appropriate factors, which enables comparing the relative effectiveness of different forms of delivery, including on-premises, off-premises commercial cloud, and off-premises access to national-scale competitive





Speed and Performance

Here I mean both the speed and responsiveness of the organization in moving to take action in response to demands, problems, and needs as well as the actual performance in situ of the (in this case) data storage and associated systems themselves.

Steps to be followed are:

- 1. Determine university need to be met
- 2. Determine type of storage and circumstances or requirements for delivery
- 3. Match need to storage type and itemize any other factors
- 4. Procure or allocate storage within a reasonable timescale

5. Verify through measurement that the need has been met

and budgetary requirements and can be kept operating within available staff time.

- Ideally this will be done as quickly as possible with a technology that meets the technical







Speed and Performance in Practice at Texas Tech

A facility like ours encounters a variety of needs ranging from small to large and supports hundreds of accounts spanning many dozens of research groups and/or classes. As with most similar academic centers, we provide all accounts with a base allocation of read/ write storage on a cluster-wide system as well as access to large amounts of scratch space (both on Lustre in our case). We also provide cluster-wide partition-specific software provisioned on read-only systems optimized for read performance. (The latter is currently done on a combination of conventional NFS, Gluster, and BeeGFS in our case.)

Lustre allows us to serve home areas with backup, work areas that are not backed up but protected from purge, and both scratch and dedicated research group areas that comprise the bulk of our cluster-wide storage. We run a separate backup service that can draw and save data from all of the above systems and save to a different storage array.

Lustre is optimized for general-purpose read/write needs, while the other systems are optimized for their functions (read performance for NFS/Gluster/BeeGFS for software distribution, local write performance for the backup system).



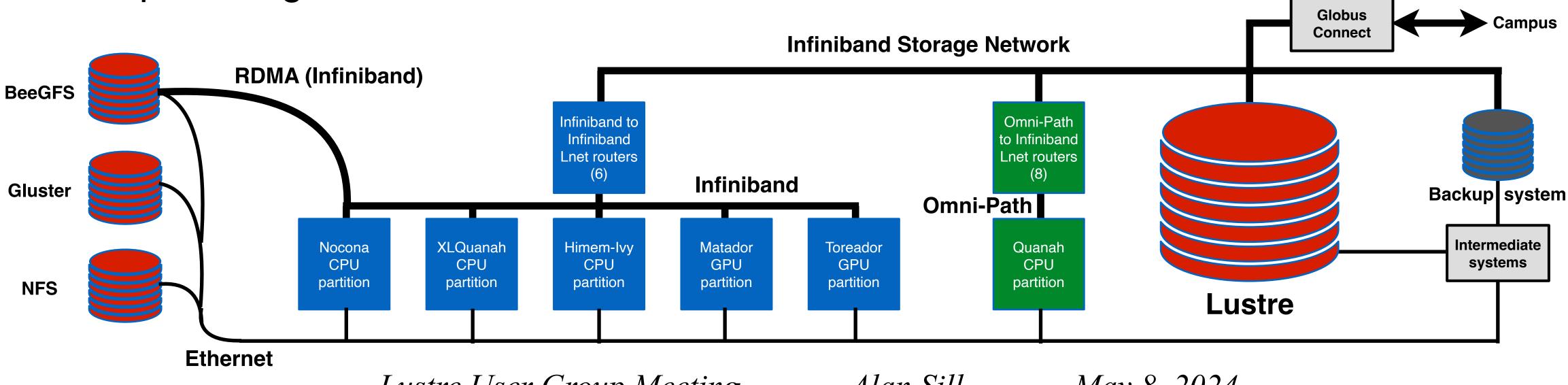




Layout of our storage system

In our local cluster, we have both Ethernet control/monitoring networks and high-speed fabrics using either Infiniband or Omni-Path, depending on the partition, for MPI traffic and access to Lustre storage. Access to the software distribution systems takes place directly through the control network for NFS and Gluster, while the BeeGFS system uses RDMA on the Infiniband-connected partitions or Ethernet on the Omni-Path connected partition. The backup system can serve all storage components directly or indirectly. Lnet routers are used to serve Lustre to all partitions by connecting them to a central

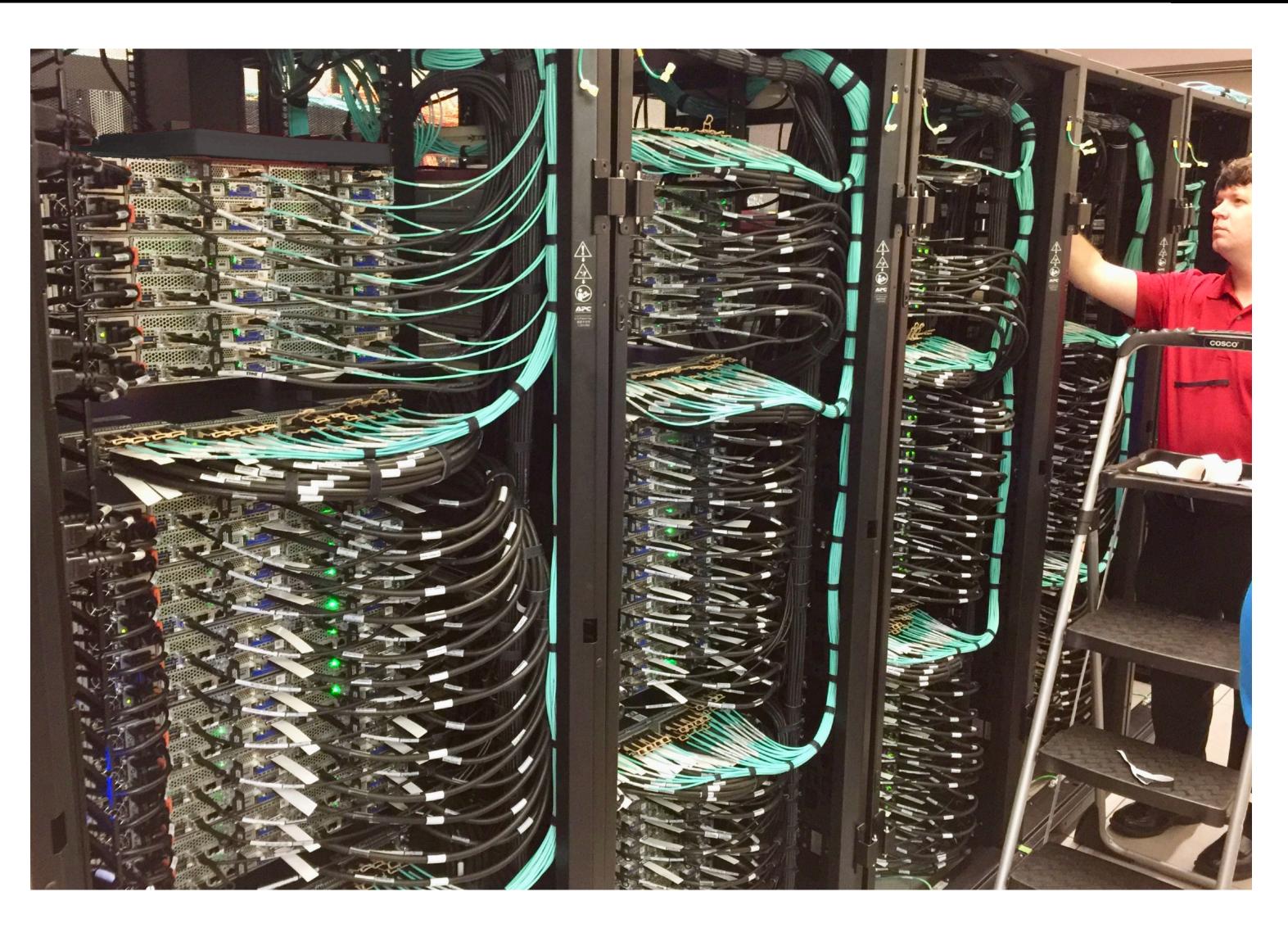
200 Gbps storage Infiniband network.





Quanah II Cluster (As Upgraded Nov. 2017)

- 10 racks, 467 Dell[™] C6320 nodes
 - 36 CPU cores/node Intel Xeon E5-2695 v4 (two 18-core sockets per node)
 - 192 GB of RAM per node
 - 16,812 worker node cores total
 - Compute power: ~1 Tflop/s per node
 - Benchmarked at 485 TF
- Operating System:
 - CentOS 7.4.1708, 64-bit, Kernel 3.10
- High Speed Fabric:
 - Intel [™] OmniPath, 100Gbps/connection
 - Non-blocking fat tree topology
 - 12 core switches, 48 ports/switch
 - 57.6 Tbit/s core throughput capacity
- Management/Control Network:
 - Ethernet, 10 Gbps, sequential chained switches, 36 ports per switch





RedRaider cluster (Delivered July 2020)

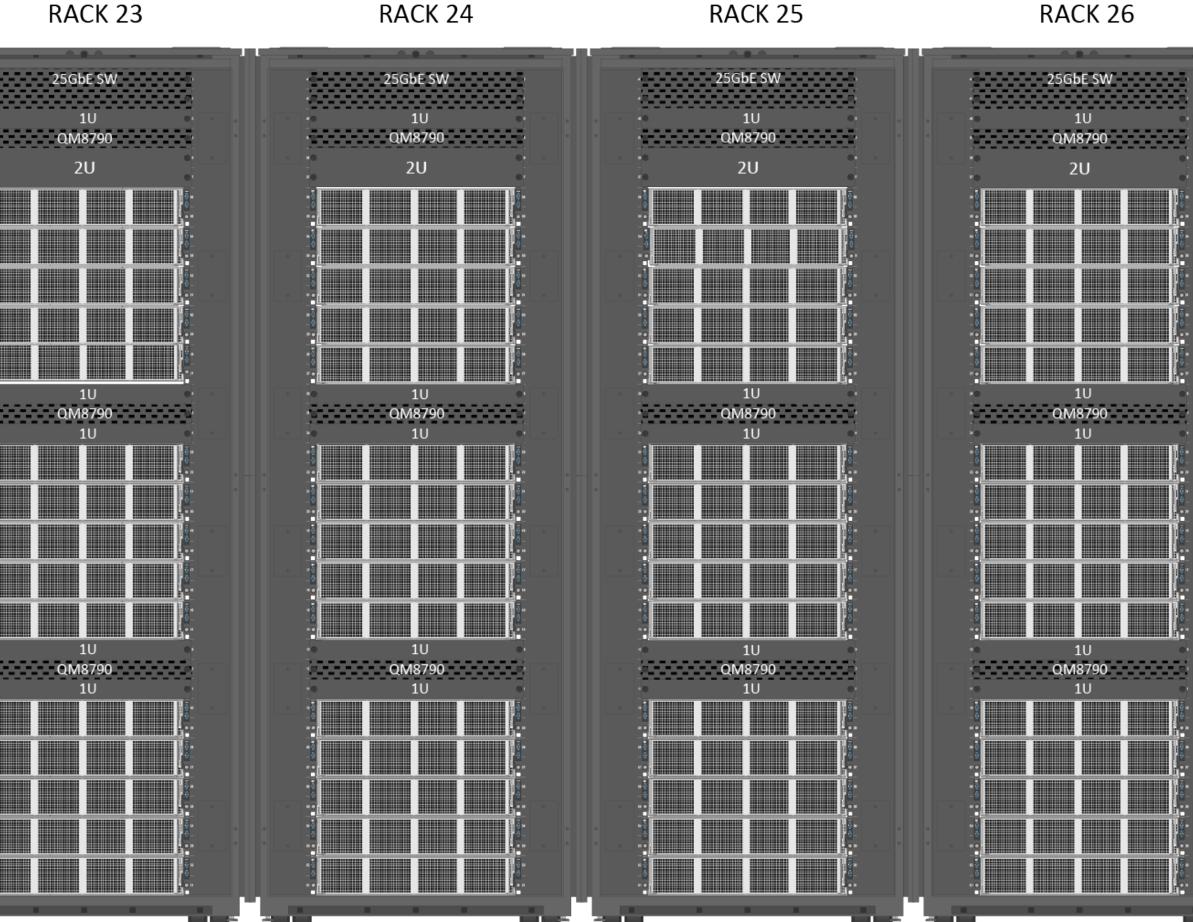
CPUs: 256 physical cores per rack unit; 200 Gbps non-blocking HDR200 Infiniband fabric GPUs: 2 NVidia V100s or 3 A100s per 2U; 100 Gbps HDR100 Infiniband to HDR200 core

RACK 20

RACK 21

RACK 22

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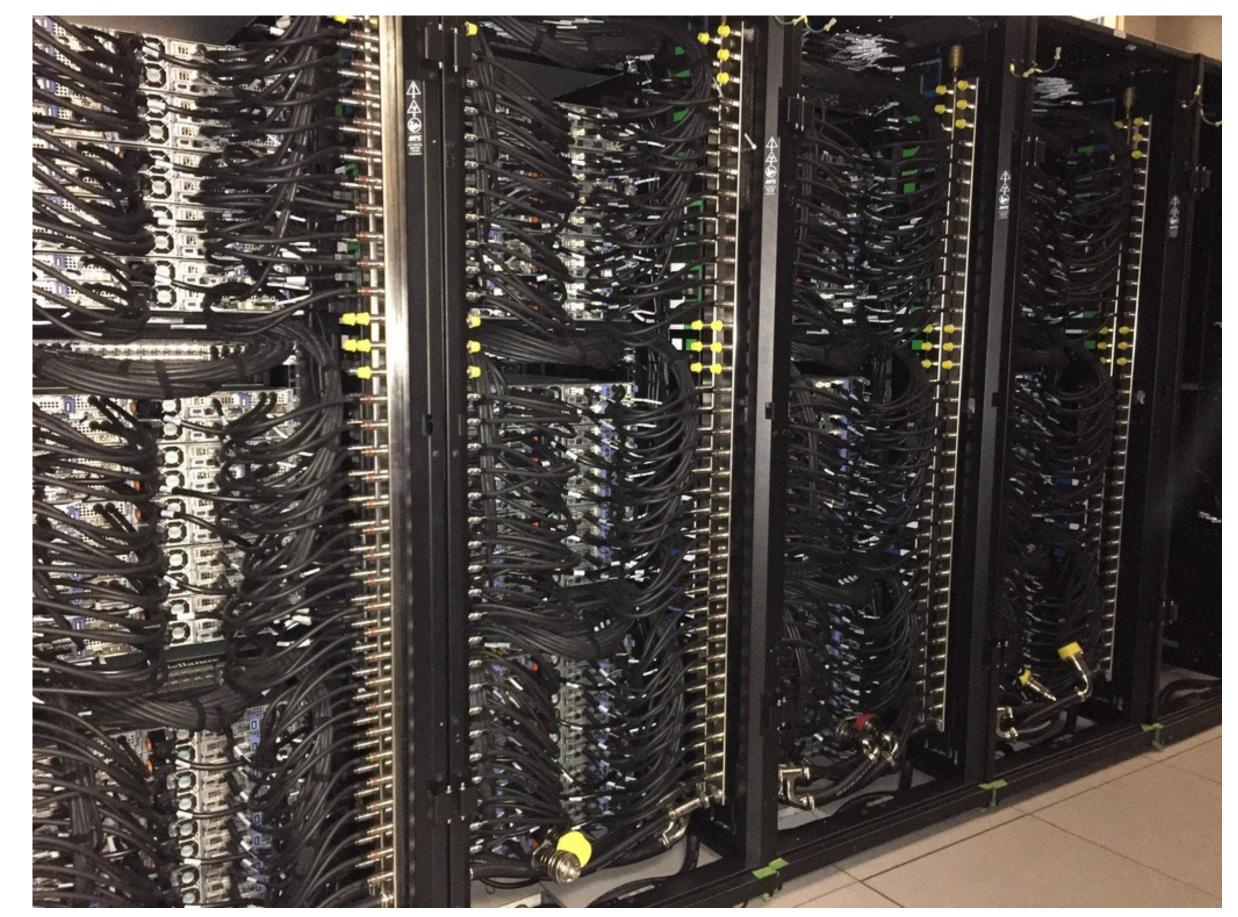


RedRaider cluster addition (2020/2021)

GPU nodes: 20 Dell R740, 2 V100 GPUs/node + 11 Dell R7525, 3 A100 GPUs/node, air cooled, 100 Gbps HDR100 CPU nodes: Dell C6525, 2 liquid cooled AMD Rome 7702, 512 GB memory/node, 200 Gbps non-blocking HDR200



Front view



Back view - CPU racks Lustre User Group Meeting — Alan Sill — May 8, 2024





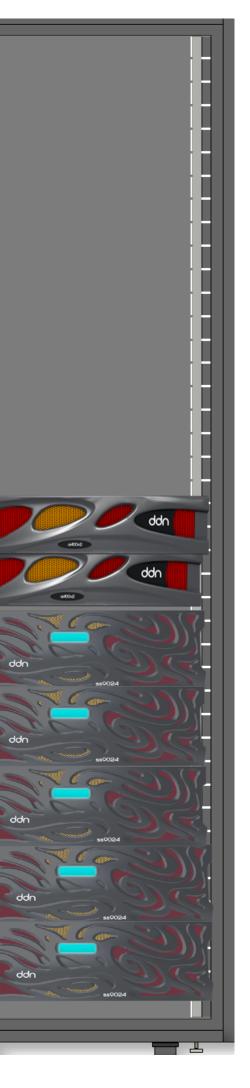


Texas Tech - DDN Storage Solution

DDN EXAScaler Storage: 1PB Usable NVME and 12.31PB Usable HDD

- (2) DDN ES400NVX2-S Controllers
- (10) SAS4 90-Drive Expansions (5 per controller)
- 12.31PB Usable HDD
- 1PB Usable TLC NVMe
- (1) ES200NVX2 for MDT
- DDN Insight Monitoring
 Application
- 5-Year Basic Hardware Support + Uplift
- 5-Year Premium Software Support
- 45U Racks Shown
- 22U used for 1 controller
 + 5 expansions per rack



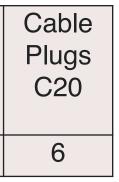


Performance Figures and Key Call Outs:

- Up to 180GB/s when configured with 48 NVME drives in (2) controllers
- Up to 6M Disk IOPS on NVME on (2) controllers
- 100GB/s on HDD
- Enclosure Redundancy
- Hot Pools Balanced

Environmentals for 2 Racks

Power, Nominal (W)	· · · ·	Heat, Nominal (BTU/	Idle	Airflow, Nominal (CFM)	Ŭ	Weight (kg)	Rack U	Cable Plugs C14
		hr)	hr)					
17026	13019	58059	44396	2605	2515	1141	46	40



Speed and performance figures in context

The DDN ES400NVX2 system described in the previous slide should give a factor of several times improvement over the performance of the previous SFA14K system we've operated for the last five years. (New system: up to 180 GB/s to NVMe or 100 GB/s to disk sustained to the cluster. Old system: up to about 40 GB/s sustained read, 32 GB/s sustained write in terms of total I/O to the cluster.) We also provide all "purchased" storage for research groups from the same hardware.

We've also upgraded our Globus Connect servers to two nodes w/ 100 Gbps each to storage and to the campus per server.

The NFS servers are in the process of switching to BeeGFS, where we hope to achieve about 90 GB/s read performance to Ethernet or ROCE for software distribution to nodes.

By themselves, these are not huge numbers. It's a *trivial exercise* to spin up cloud-based Lustre systems these days that can achieve terabytes/second of throughput, but this costs money. The main point for achieving these values on an academic setting is to be able to deliver them on a <u>continuous stable basis</u> within a <u>budget that the campus can afford</u>.









Provenance and Protections

Increasingly, research is being conducted in settings in which the funding agency places significant restrictions for required protections to be in place (CMMC, CUI, HIPAA, etc.) and campuses need to put appropriate systems in place to handle these.

Such systems are not trivial to design and implement, in many cases are not optional, and come with definite auditing, certification, and reporting requirements.





Links for research cyberinfrastructure and data security topics

High-Performance Computing Security Working Group I Computer Security Resource Center I NIST <u>https://csrc.nist.gov/projects/high-performance-computing-security</u>

Executive Order 13702 established the National Strategic Computing Initiative (NSCI) to maximize the benefits of high-performance computing (HPC) for economic competitiveness and scientific discovery.

Regulated Research Community of Practice https://www.regulatedresearch.org

Community group that includes a Slack channel, organizes webinars and workshops for exchange of information, etc.

Trusted CI: The NSF Cybersecurity Center of Excellence https://www.trustedci.org

A National Science Foundation Cybersecurity Center of Excellence, Trusted CI collaborates with NSF-funded research organizations to address their unique cybersecurity challenges.





Challenges that come from these considerations

- 1. Provide data processing and handling needs to an increasing number of departments and fields of study.
- 2. Address the overwhelming interest in machine learning, data mining, large language modeling, and other related applications that have become known widely as "AI".
- 3. Handle the growing needs for data volume, data transparency and labeling, data protection, access controls, sharing, publication support and archival, backup, permanence, protection, regulation, etc.
- 4. Find funding models that can achieve the above within organizational capabilities.
- 5. Find ways to address the power, cooling, space, and staffing needs for on-premises resource and/or equivalently to provide for cloud-based resource alternatives.

As the need to serve an increasing portion of the academic and research computing activities grows, all of the organizational capabilities are increasingly under challenges:



Challenges viewed more globally

It is not just the academic and research sector that is encountering these challenges. In fact, as most know, academic and research computing has become dwarfed in terms of scale in comparison to the size of industry and commercial deployments.

Our research with CASC has shown however that most organizations with on-campus centers find them much cheaper to operate on their own so far compared to the cost of using commercial cloud services for bulk computing and data processing at scale.

As the cost and scale of these resources grow, electricity (and hence, carbon emissions) impact, cooling, data center design) have become significant limiting factors for both commercial and academic data centers. Academic centers have routinely reached many megawatts, and commercial data facilities are being implemented routinely at the many hundreds of megawatts to gigawatts scale.

This cannot continue unchecked. We have to do something to control the cost and carbon impact of data center deployments. Here at Texas Tech we have several projects either deployed or underway to address this issue directly. Ask me if you want more details!



Conclusions

support for academic and research computing, data handling, and services:

- 1) How do they serve the *core functions* of the university or institution?
- 2) What is the *return on investment* in terms of those core functions?
- 3) With what *speed and performance* can needed services can be delivered?
- 4) What *provenance and protections* need to be applied to the services?

cautions for what is coming in the near future. In summary:

In summary, we have considered four basic questions that need to be answered for delivery of

- I've provided details on the above both in general terms and with examples from how we approach them at Texas Tech, and offered some questions and warnings about trends we are seeing and
- Al and data growth present challenges that I think most campuses are not equipped to meet.
- The trend to growing power and cooling requirements needs to be met head-on with increasing research to address these requirements in both academic and industry settings.
 - Lustre User Group Meeting Alan Sill May 8, 2024



