

Next Generation Networks and Systems for Data Intensive Science



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Network Research Problems + Challenges for DOE Scientists Workshop Bethesda, February 1 2016

Entering a New Era of Technical Challenges as we Move to Exascale Data and Computing



- The largest science datasets today, from LHC Run1, are 300 petabytes
 - Exabyte datasets are on the horizon, by the end of Run2 in 2018
 - These datasets are foreseen to grow by another 100X, to the ~50-100 Exabyte range, during the HL LHC era from 2025
- The reliance on high performance networks will thus continue to grow as many Exabytes of data are distributed, processed and analyzed at hundreds of sites around the world.
- As the needs of other fields continue to grow, HEP will face increasingly stiff competition for the use of large but limited network resources.



A New Era of Exploration and Discovery in Data Intensive Sciences: Challenges



- Scale of Datasets and Network Traffic [LHC view]
 - Data Stored: from 300 PBytes now to ~1 Exabyte by 2019
 - Traffic Flows: from 20-50 Gbps (with peaks to 90 Gbps) now; More sites and diverse paths; 100G+ flows "when possible"
 - Aggregate Transfers (WLCG): 50 PBbytes/month in Fall 2016; Projects to 1 Exabyte/month by ~2020 to 10 EB/Month by ~2024
- Complexity: Of diverse workflows, global topology, flow paths
 - Workflow: Organized dataset transfers, job output files, object collection access
 - Matching Jobs to Data: Redirection of data as needed
 - Of global topology (peerings and interconnections): LHCONE example
- Reactive, sometimes chaotic operations
 - Lack of network awareness by applications and users
 - Highly varied level of network capability among sites and regions
 - Lack of monitoring, interaction, feedback; moderation of user behavior
- Drivers: Bottom Up and Top Down Combined
 - Mission Need: LHC to LSST to Genomics; the Exascale Imperative
 - Technology and Opportunity Drivers: Low cost servers (CPU, storage) + apps capable of 100-500 Gbps with 100G NIC(s) and FDT; new memory, storage, OS

Complex Workflow: the Flow Patterns Have Increased in Scale and Complexity, even at the start of LHC Run2

WLCG: 170 Centers in 40 Countries. 2 Million Jobs Per Day



WLCG Dashboard Snapshot Sept-Oct. Patterns Vary by Experiment

Caltech and Partners Terabit/sec SDN Driven Agile Network: Aggregate Results

900 Gbps Total Peak of 360 Gbps in the WAN



100g01.sc15.caltech.edu = 100g02.sc15.caltech.edu = 400g01 = 400g02 = 400g03 = 400g04 = C144.1009.sc15.org E140.1248.sc15.org = E141.1248.sc15.org = E142.1248.sc15.org = fiu-100g = localhost = premiotest sandy01-gva.ultralight.org = sandy03-gva.ultralight.org = sc15-austin.sc15.org = sgi01 = sgi02 = srcf-sc15-d1.stanford.edu

MonALISA Global Topology



Single port smooth Flows up to 170G; *120G over the WAN.* With Caltech's FDT TCP Application http://monalisa.caltech.edu/FDT

ORNIA



A stepping stone to our joint future: for data intensive sciences

The LHC: Spectacular Performance

Data Complexity: The Challenge of Pileup



Run2 and Beyond will bring:

- Higher energy and intensity
- Greater science opportunity
- Greater data volume & complexity
- A new Realm of Challenges



~3.5 X 10¹⁵ pp Collisions 1M Higgs Bosons created in Run 1



~50 Vertices, 14 Jets, 2 TeV

Average Pileup Run 1 21 Run 2 42 Run 3 53 HL LHC 140-200

Achieving a New Era of Exploration and Discovery Rising Challenges and Needs



- It is getting too easy to match the capacity of production networks today, with 1000s of compute nodes, or with a very few well configured DTNs
- Exhaustion of network resources may come before the next generation
- The intensity of usage will increase as the LHC program progresses; The outlook is for increasingly chaotic operations unless:
- Network awareness of users and applications is raised
- Interaction and feedback among user applications and network operations is implemented: getting users and the network "on the same side"
 - Service Classes including preferred service for those that plan, interact and well-use allocated resources
- Greater Predictability (of transfers in progress, scheduled and planned) is achieved, through intelligent network services and pervasive monitoring
- Greater intelligence and agility is implemented in the network:
 - Short term: path selection, flow steering, load balancing, allocation of scarce resources; strategic rebalancing
 - Longer term: managing resource allocations, identifying "reliable" requestors, fair-sharing over week/month/year
- Bottom Line: A real-time end-to-end system with a top down view, pervasive monitoring + a management paradigm (goals, strategy and tactics) is needed



Use of high capacity reliable networks opens up the "phase space" of available and affordable resources



辈 Fermilab

15. April 2015

Gabriele Garzoglio, Oliver Gutsche I CHEP2015: Diversity in Computing Technologies and Strategies for Dynamic Resource Allocation

Provisioning for Peak Demands

Vision of short turn-around times for HEP major workflows

- Short latencies in particular in analysis workflows are important for science efficiency
- Using resources from a larger pool when they are needed, should also result in more cost-effective solutions
- Separating the processing and storage services allows them to scale independently
- e.g. ATLAS and CMS are looking at ways to double available resources for periods of time, Using Amazon services
 - CMS: 56k Core MC production now underway



Provisioning for peak requires that
we use pooled resources
Clouds and/or large HPC Centers!

Achieving a New Era of Exploration and Discovery Elements for Success



- Bringing basic capability to the community: Beyond "best practices"
 - Workshops and field deployments of well configured DTNs + applications
- Reducing heterogeneity: bringing all areas to a minimum level
 - Identification and resolution of problem sites, links, regions
- Raising network awareness
 - A paradigm of "interaction leads to improved service"; non-interacting applications/users get best effort service, mapped onto a limited fraction of the available network resources
 - Interaction is imperative for users/groups that have a major impact on the networks and/or require priority service on demand
- Development of new "real time systems, driven by application / site/ network interactions, with true end-to-end operations
 - Agent based architectures with great resilience and adaptability
 - Monitoring systems with great scalabilility, pervasiveness, MTBF
- SDN is a natural pathway
 - Intent-based networking will ease the task for some users; but greater transparency implies greater intelligence "under the hood"
 - Which SDN: ODL, ONOS; OpenvSwitch, Openstack, or other ?
 - A powerful, rapidly advancing direction: but highly diverse and fluid

Achieving a New Era of Exploration and Discovery Concepts and Issues



- System Architectural Concepts: Open systems with simple characteristics versus more intelligent, deterministic, predictable systems that are internally more complex, including stateful "end to end system services". Examples
 - Emerging network operating systems to manage network/site/user interactions based on intents
 - Real-time distributed systems: technically possible but difficult outside the single project "domain"
 - Monitoring systems that can track end-to-end operations: require sufficient data access across multiple sites and domains
 - Information Centric Networks: how much state is needed/wanted for data discovery, caching & routing as a function of data transaction size
- Network system/user interaction models: trading engagement and rule-based behavior for resources beyond the lowest common denominator
- Choices: diversity versus emerging standards and the ability to build on a common base. Choices that are more than technical survival of the fittest.
- Resource Sharing: Mission oriented tasks versus general service; degree of mission orientation and hence the resource allocation profile: varying by network, region and domain
- Consistent operations: high water marks for individual + aggregate large flows

Vision: Next Gen Integrated Systems for Exascale Science: Synergy ⇒ a Major Opportunity

Exploit the Synergy among:

- 1. Global operations data and workflow management systems developed by HEP programs, being geared to work with *increasingly diverse and elastic resources to respond to peak demands*
 - Enabled by distributed operations and security infrastructures
 - Riding on high capacity (but mostly still-passive) networks



- 2. Deeply programmable, agile software-defined networks (SDN) Emerging as multi-domain network "operating systems"
 - + New network paradigms focusing on content: from CDN to NDN
- 3. Machine Learning, modeling and simulation, and game theory methods Extract key variables; optimize; move to real-time self-optimizing workflows
- * The Watershed: A new ecosystem with ECFs as focal points in the global workflow; meeting otherwise daunting CPU needs

Achieving a New Era of Exploration and Discovery Mechanisms and Choices: What is the Role ?



- Dynamic Circuits: How hard or flexible the bandwidth guarantees ? How dynamic in time and capacity ?
- Role of Slices: Who can (qausi-permanently) reserve a slice ?
- Flow Steering: Classes of work definition and parameters; Authorization, priority; Dynamism: How often and how extensive ?
- Load balancing: Tactical and strategic; Dynamism questions as above
- Protocols: Policies and operations on inefficient or unfriendly protocols, and "inefficient" users; Protecting a valuable resource
- Layer 1 as well as Layer 2: Where and when
- For several of the above: guidelines on agility versus stability
- Coexistence of heterogeneous domains: with varying architecture, topology, technologies, performance, and Policies
- New "stateful" models of use and sharing: "Cost" based, quota based, role/priority based; top level metric based
- Effective Metrics: Throughput, resource usage, average + maximum time to completion, overall user-organization "satisfaction". What is optimal ?



THANK YOU!

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ADDITIONAL ILLUSTRATIVE SLIDES FOLLOW

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Location Independent Access: Blurring the Boundaries Among Sites + Analysis vs Computing

Once the archival functions are separated from the Tier-1 sites, the functional difference between Tier-1 and Tier-2 sites becomes small [and the analysis/computing-ops boundary blurs]

Connections and functions of sites are defined by their capability, including the network!!





Entering a new Era of Exploration and Discovery in Data Intensive Sciences



- We are entering a new era of exploration and discovery
 - In many data intensive fields, from HEP and astrophysics to climate science, genomics, seismology and biomedical research
- The largest data- and network-intensive programs from the LHC and HL LHC, to LSST and DESI, LCLS II, the Joint Genome Institute and other emerging areas of growth face unprecedented challenges
 - In global data distribution, processing, access and analysis
 - In the coordinated use of massive but still limited CPU, storage and network resources.
- High-performance networking is a key enabling technology for this research: global science collaborations depend on fast and reliable data transfers and access on regional, national and international scales





The Future of Big Data Circa 2025: Astronomical or Genomical ? By the Numbers

PLoS Biol 13(7): e1002195. doi:10.1371/journal.pbio.1002195

Domains of Big Data in 2025. In each, the projected annual and storage needs are presented, across the data lifecycle

Basis: 0.1 to 2B Humans with Genomes, replicated 30Xs;

+ Representative Samples of 2.5M Other Species' Genomes

Data Phase	SKA	Twitter	YOU TUBE	GENOMICS	HL LHC
Acquisition	25 ZB/Yr	0.5–15 billion tweets/year	500–900 million hours/year	1 Zetta-bases/Yr	
Storage	1.5 EB/Yr	1–17 PB/year	1–2 EB/year	2-40 EB/Yr	2-10 EB/Yr
Analysis	In situ data Reduction	Topic and sentiment mining	Limited requirements		
	Real-time processing	Metadata analysis		Variant Calling 2 X 10 ¹² CPU-h	
	Massive Volumes			All-pairs genome alignment 10 ¹⁶ CPU-h	<mark>0.065 to 0.2 X</mark> 10 ¹² CPU Hrs
Distribution	DAQ 600 TB/s	Small units of distribution	Major component of modern user's bandwidth (10 MB/s)	Many at 10 MBps Fewer at 10 TB/sec	DAQ to 10 TB/s Offline ~0.1 TB/s

Conclusion: Genomics Needs Realtime Filtering/Compression Before a Meaningful Comparison Can Be Made







SDN-driven flow steering, load balancing, site orchestration Over Terabit/sec Global Networks

Consistent Operations with Agile Feedback: Supporting Major Science Flows Compatible with other Traffic

29 100G NICs Two 4 X 100G DTNs Two 3 X 100G DTNs 9 32 X100G Switches

Caltech HEP & Partners. Open Daylight Controller

SC15: SDN Driven Next Generation Terabit/sec Integrated Network for Exascale Science



SDN-driven flow steering, load balancing, site orchestration Over Terabit/sec Global Networks

Consistent Operations with Agile Feedback: Major Science Flow Classes Up to High Water Marks

PetaByte Transfers to and From the Site Edges of Exascale Facilities With 400G DTNs

Caltech HEP & Partners. Open Daylight Controller

Mellanox and Qlogic 100G and Mellanox N X 100G NIC Results





Using Caltech's FDT TCP Application http://monalisa.caltech.edu/FDT

Entering a New Era of Technical Challenges as we Move to Exascale Data and Computing

- Beyond network capacity and reliability alone, the keys to future success are next generation systems able to:
 - Respond agilely to peak and shifting workloads
 - Accommodate a more diverse set of computing systems from the Grid to the Cloud to HPC
 - Coordinate the use of globally distributed computing and storage, and networks that interlink them
 - In a manner compatible across fields sharing common networks
- The complexity of the data, and hence the needs for CPU power, will grow disproportionately: by a factor of several hundred during the same period







CMS at SC15: Asynchronous Stage Out 3rd Party Copy Demonstration

□ All control logic in ASO:

- Group multiple file transfers per link
- Controls number of parallel transfers
- Transparent for ASO integration
- Only FDT daemon has to be installed on storage site
- Tests between end-hosts at Caltech, Umich, Dell booths and outside: FIU, Caltech, CERN, Umich
- PetaByte transfers from multiple sites to multiple locations



LSST + SKA Data Movement Upcoming Real-time Challenges for Astronomy



□ Lossless compressed Image size = 2.7GB
 (~5 images transferred in parallel over a 100 Gbps link)
 □ Custom transfer protocols for images (UDP Based)
 □ Real-time Challenge: delivery in seconds to catch cosmic "events"
 □ + SKA in Future: 3000 Antennae covering > 1 Million km2;
 15,000 Terabits/sec to the correlators ≠ 1.5 Exabytes/yr Stored

CMS Offline Computing Requirements HL LHC versus Run2 and Run1 [*]



HEP Collider HPC Use, Prospects and Wishes Tom Lecompte (Argonne) at the Exascale Workshop

Computing to reach the Science Goals: Argonne LCF Use



An excellent very promising start. A lot of work remains

Key Developments on the HEP Side Enabling the Vision: Coherent Parallel Architectures

We need to recast HEP's code and frameworks for the highly parallel, energy efficient architectures (GPU, Knights Landing, etc.) of modern HPC systems Significant progress in specific HEP areas exists

CMS threaded memory-efficient concurrent framework for multicore CPUs



90% efficient with 16 threads reco code is 99.3% parallel Number of Cores

ATLAS generators have successfully run on (all of) MIRA (100M events in 1M threads); Looking towards Aurora [Tom LeCompte +]

Exascale "CSN" Ecosystems for Next-Generation Data Intensive Science

- The opportunity for HEP (CMS example):
 CPU needs will grow 65 to 200X by HL LHC
 - Dedicated CPU that can be afforded will be an order of magnitude less; even after code improvements on the present trajectory
- DOE ASCR/HEP Exascale Workshop:
 - Identified key opportunities for harnessing the special capabilities of ECFs
 - Exposed the favorable outlook and issues for HEP to take this key step + meet the needs
 - Highlighted the Network Dimension
- Important added benefits to HEP + ASCR, the facilities, programs and the nation
 - Shaping the future architecture and operational modes of ECFs
 - Folding LCFs into a global ecosystem for data intensive science
 - Developing a "modern coding workforce"
 - Enabling many fields to "think out of the box"



A favorable HEP platform:

 LHC experiments are gearing their S&C operations for more flexible use of diverse resources: Grid, Cloud, HPC

LCF-Edge Data Intensive Systems (LEDIS) **Operational Model**

- □ In the context of a new HEP LCF ESnet partnership for Joint system and architecture development
- Data brought to LCF edge ~petabyte chunks: Delivery in ~2 hrs at 1 Tbps Far enough in advance: chunks ready and waiting in a buffer pool
- Using secure systems at the site perimeter: Security Efforts (human and AI) can be focused on a limited number of entities (proxies) Keeping manpower + risk at acceptable levels Content delivery network: deliver data quickly and efficiently by placing data of interest close to its clients
- Multiple chunks for different stages of the workflow Each chunk's provenance + attributes identified
 - **Examples:** Input/Output Data size, memory, CPU to IO ratio; delivery deadline, authorization level
- Enables matching to appropriate HPC subsystems, to meet the needs while operating at high efficiency

T. Wenaus BNL/ATLAS

* Conceptual Extension: Caching in the Network, or at nearby HEP Lab Sites; as in "Data Intensive" CDNs (or NDNs)

Adapting to the future Internet architecture that may emerge

Key Developments from HPC Facility Side Enabling the Vision: ECF Architecture

- Developing appropriate system architectures in hardware + software that meet the needs
 - Edge clusters with petabyte caches
 - Input + output pools: ~10 to 100 Pbytes
 - * A handful of proxies at the edge
 - * To manage and focus security efforts
 - Identifying + matching HEP units of work to specific sub-facilities adapted to the task
 - Extending Science DMZ concepts
 - Enabling 100G to Tbps SDNs with Edge/WAN
 Coordination + DTN Autoconfiguration
 - Site-Network End-to-End Orchestration
 - * Efficient, smooth petabyte flows

Dynamic agile systems that learn to adapt to peaking workloads

Convergence and Collaboration Tackling the Larger Mission

34

- Empowering Data Intensive Science across multiple fields through efficient, manageable use of national & global infrastructures up to high occupancy levels, including multi-pathing
- Using SDN-driven coordinated use of computing, storage and Network resources for efficient workflow
- Enabled by Pervasive End-to-end Monitoring
- Consistent Operations: Networks ⇔ Science Programs; with feedback
- Key Concepts and Technologies for Success:
 - Dynamic circuits for priority tasks, with Transfer Queuing, Deadline scheduling, Efficient worldwide distribution and sharing
 - Classes of Service by flow characteristics, residency time
 - Load balancing, hotspot resolution, strategic redirection
 - State-based error propagation, localization, resolution
 - SDN driven Intent-based deep site-network orchestration functions
 - System Level Optimization Using Machine Learning

SDN in SDN-NGenIA and SENSE

Ideas Building on Caltech/Esnet/FNAL Experience

Vision: Distributed computing environments where resources can be deployed easily and flexibly to meet the demands of data-intensive science, giving transparent access to an integrated system of enormous computing power

SDN is a natural pathway to this vision: separating the functions that control the flow of network traffic, from the switching infrastructure that forwards the traffic itself through open deeply programmable "controllers".

With many benefits:

- Replacing stovepiped vendor HW/SW solutions by open platform-independent software services
- Imagining new methods and architectures
- Virtualizing services and networks: lowering cost and energy, with greater simplicity

opennetworking.org

A system with built in intelligence Requires excellent monitoring at all levels

SC15: SDN Driven Terabit/sec Live OF Network Topology for Directing Flows

SENSE: SDN for End-to-end Networked Science at the Exascale ESnet Caltech Fermilab Argonne Maryland

Mission Goals: Significantly improve endto-end performance of science workflows Enabling new paradigms: creating dynamic distributed 'Superfacilities'. **Comprehensive Approach:** An end-to-end SDN Operating System (SENOS), with:

SENSE SDN Control Plane Architecture for End-to-End Orchestration

Intent-based interfaces, providing intuitive access to intelligent SDN services
 Policy-guided E2E orchestration of resources
 Auto-provisioning of network devices and Data Transfer Nodes

Network measurement, analytics and feedback to build resilience 37

Key Developments from the HEP Side Enabling the Vision: Machine Learning

- Applying Deep Learning + Self-Organizing systems methods to optimize LHC workflow
 - Unsupervised: extract key variables/functions
 - Supervised: to derive optima
 - Iterative and model based: to find effective metrics and stable solutions [*]
- Complemented by game theory methods, modeling and simulation
- Shown to be effective to solve traffic, communications and workflow problems
- Starting with logged monitoring information
- Progressing to real-time agent-based pervasive monitoring
- [*] T. Roughgarden (2005). Selfish routing and the price of anarchy

Self-organizing neural network for job scheduling in distributed systems

Computing Operation Automation Example of a Model (State Machine)

Fully automate handling of production request

- production requests
- Pre-defined simple rules of placement
- Automation of sanity check and final delivery
 - Amount of operator work reduced
- Now possible to handle larger, more diverse resources smoothly

Computing Optimization R&D

Machine Learning Coupled to Modeling and Simulation

Learn complex models using deep learning with monitoring data and the chosen metric(s)

- Use simulations together with game theory techniques or a reinforcement learning method to find optima
 - Variations: evolve towards the metrics yielding stable solutions with good throughput
 - Balancing among max throughput, balanced resource use, predicability of time to completion (predictable workflow) etc.

Steering computing, storage and network elements like robot arms

Networks for HEP and Global Science Our Journey to Discovery

- Run 1 brought us a centennial discovery: the Higgs Boson
- Run 2 will bring us (at least) greater knowledge, and perhaps greater discoveries: Physics beyond the Standard Model.
- Advanced networks will continue to be a key to the discoveries in HEP and other data intensive fields of science and engineering
- Technology evolution might fulfill the short term needs
- Near Term Challenges: A new net paradigm including the global use of circuits will need to emerge during LHC Run2 (in 2015-18)
- New approaches + a new class of global networked systems to handle Exabyte-scale data are needed [LHCONE, DYNES, ANSE, OIIMPS; SENSE+SDNNGenIA]
- Worldwide deployment of such systems in ~2020-24 will be:
 - Essential for the High Luminosity LHC HL-LHC
 - A game-changer, with global impact, shaping both research and daily life

Data Intensive Exascale Facilities for Science Deep Implications

Adapting Exascale Computing Facilities to meet the highest priority needs of data intensive science, including high energy physics as a first use case (to be followed by others) will have profound implications:

- Empowering the HEP community to make the anticipated next and future rounds of discoveries
- Encouraging, and provoking the US scientific community to Think "top down" (Out of the Box) as well as "bottom up"
 - Envisioning a new scale; new applications, methods; and a new overall approach to science
 - Especially: in the face of an emerging discovery and the exploration of its aftermath

HEP is a natural partner and thought co-leader in this process, and in the achievement of this goal

Data Intensive Exascale Facilities for Science Deeper Implications

- Bringing these facilities into the ecosystem of globally distributed information and knowledge sources and sinks
 - □ The hallmark of science, research and everyday life this century
- Will open new avenues of thought and new modes of the pursuit of knowledge in the most data intensive fields
 - By responding to petascale inquiries on human time scales, irrespective of location
 - **Bringing our major networks, once again, into sharp focus**
- This will broaden the function and architecture of ECFs and ultimately shape them in future generations
 - □ While also shaping the leading edge of "modern computing and networking"

And place the US science community in a new position of leadership Being the first to cross this conceptual threshold

THANK YOU!

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