HEPiX Spring 2019 Summary

https://indico.cern.ch/e/hepix-spring2019

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Hosted by University of California in San Diego at San Diego Supercomputing Center

HEPiX

Future plans

Working groups

Challenges

CERN IHEP DESY INFN PIC NIKHEP RAL FZU BNL …

2x / year

AGLT2 KIT GSI TRIUMF FNAL KEK IN2P3 NERSC …

Recent work

Status reports

Experiences

https://www.hepix.org

Andrei

Spring 2019 Meeting and General HEPiX News
Security and Networking
Basic IT Services
Site Reports

Piotr

Computing and Batch Services
Storage and Filesystems
Miscellaneous

Quentin

Grid, Cloud and Virtualisation
IT Facilities and Business Continuity
End-User IT Services and Operating Systems

HEPiX 2019 Spring in numbers
88 registered participants

39 from Europe
31 from North America
 4 from Asia
14 from companies/corporate sponsors

HEPiX 2019 Spring in numbers
64 contributions

Site Reports (19)
Networking & Security (7)
End-User IT Services & OS (3)
Storage & Filesystems (10)

Computing & Batch Services (7)
IT Facilities & Business Continuity (7)
Basic IT Services (2) Misc. (1)
Grids, Clouds & Virtualisation (8)

35+ years of operational history

SDSC is home to:
- COMET supercomputer
- Open Science Grid
- Scherlock Cloud on AWS (burst to cloud)

Users:
- Main users: biology, neuroscience
- Small HEP community
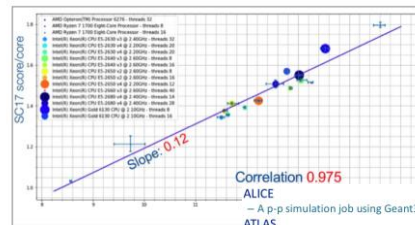
Computing and Batch Services

- Performance benchmarking and optimization for grid computing

- WLCG Site infrastructure developments

- Computing with Jupyter notebooks

Computing and Batch Services
Performance benchmarking and optimization for computing

Presentation from HEPIX Benchmarking working group:
- Benchmarks to classify hardware (single hosts) running in WLCG
- HS06 benchmark obsolete, evaluating SC2017 (similar results). New benchmarks based on example jobs provided by experiments. Gitlab group hep-benchmarks for contributions

Analysis of fair-sharing in grid from IN2P3—proposals to address and fine- tune batch policy:
- Analysis and proposals on optimisation and configuration of queues to speed-up local jobs without harming grid jobs (UGE Univa Grid Engine used - looking also at HTCondor. Storage GPFS, HPSS, iRODS, dCache, XrootD)

Redefinition of the scheduling queues

Workload	Scenario	Average	Percentiles			Maximum
			50th	75th	90th	
Grid	Baseline	1h 10m	0s	8m 18s	1h 18m	15d 21h 54m
	Modified	1h 45m	0s	14m	2h 2m	14d 4h 33m
Local	Baseline	2h 3m	4m 30s	1h 40m	6h 40m	11d 21h 41m
	Modified	1h 58m	8s	1h 10m	6h 20m	4d 19h 6m

Quota Relaxation

| Workload	Scenario	Average	Percentiles			Maximum
			50th	75th	90th	
Grid	Conservative	1h 53m	0s	16m	2h 21m	13d 15h 21m
	Extreme	1h 57m	4s	17m 41s	2h 47m	14d 4h 41m
Local	Conservative	1h 39m	2s	45m 40s	5h 8m	3d 16h 58m
	Extreme	1h 14m	1s	21m 55s	2h 30m	3d 23h 11m

Computing and Batch Services

Site infrastructure developments

Presentation from DESY on infrastructure evolution for future online processing requirements:
- With future evolution current workflow (Detector -> GPFS -> offl. Ana -> tape) will not be efficient.
- Evaluating online analysis with ASAP:0 system: Detector -> Reduction Techniques (no raw data stored) -> Storage -> Online Analysis on data with Jupyter Notebooks
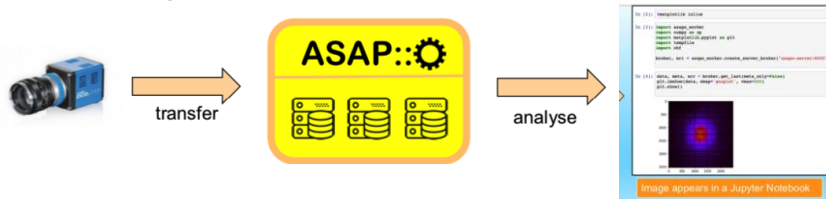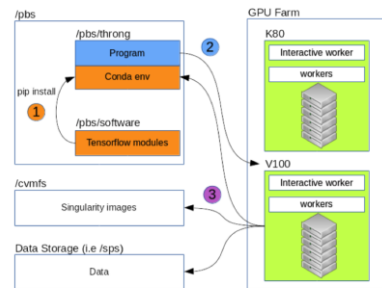
Presentation from Swiss HPC Tier-2 (CSCS):
- Investigating use of HPC (including GPUs) dominantly for HL-LHC with dCache and GPFS scratch space
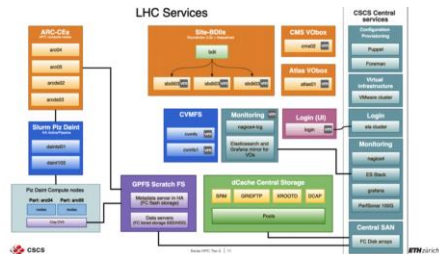
Presentation from IN2P3 on GPUs farm:
- Investigating use of GPUs with Tensorflow on grid GPU farm, with containers (Singularity)
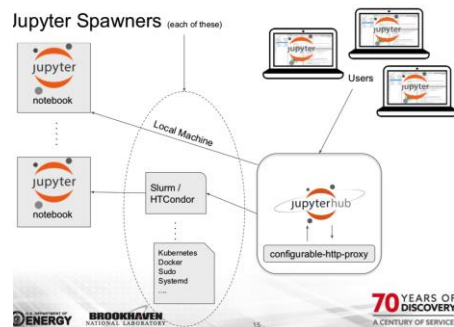
Computing and Batch Services
Computing with Jupyter notebooks

Presentation from Brookhaven National Laboratory on Notebooks integrations:

- Integration of Jupyter Notebooks into their computing environment (Slurm/HTCondor - interactive submission of set of jobs or scheduling notebook as single job)
- Notebooks scheduled on HTC/HPC resources

Presentation from CERN IT-DB-SAS on Notebooks, Spark and RDataFrame:

- Challanges and motivation for integration of Jupyter/Spark Notebooks with K8s Container Service, compared to existing on-premise Hadoop
- Interactive analysis for physics with Distributed RDataFrame on real user analysis example (Proton's Elastic Scattering)


```
df = RDataFrame(dataset)

df2 = df.Filter('x > 0')
        .Define('r2', 'x*x + y*y')

h = df2.Histo1D('r2')
g = df2.Graph('x', 'y')
```
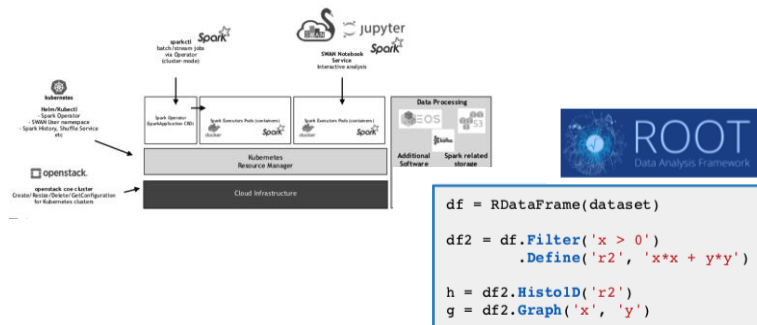
Storage and Filesystems

- Updates on Software

- Site infrastructure developments and updates

Storage and Filesystems
Updates on Software

Presentation from OpenAFS:
- 1.8.X is new stable release of OpenAFS (platform support for new releases of linux, fixes)
- 1.6.X old stable will be still supported and no EOL so far (backports from 1.8.x)
- 1.8.3 will soon be released (platform support and maintenance fixes)

Presentation from WEKA.IO:
- presented a GPU-optimized storage filesystem that outperforms other popular filesystems on data processing on GPUs (storage in S3-compatible systems)
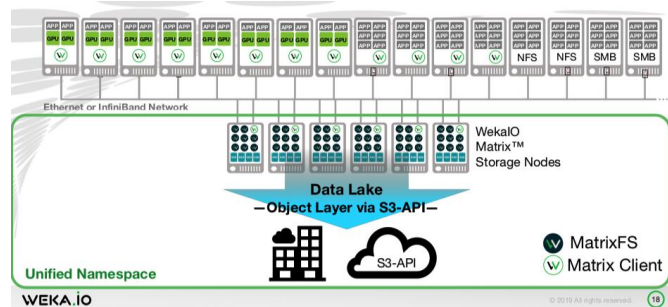
Presentation from FZU on Disk Pool Manager:
- DPM old code will be discontinued, moved to DOME (Disk Operations Management Engine). DPM Sites should move to DOME

Storage and Filesystems
Updates on Software

Presentation from HEP sites on OSiRIS pilot:
- <u>Software-defined storage infrastructure for transparent, high-performance access to storage infrastructure</u> (cred mgmt, user mgmt/provisioning, monitoring)
- <u>Pilot on multi-institutional Ceph-Posix/Ceph-S3 Cluster</u> spanning University of Michigan, Michigan State University, Wayne State UNiveristy and Van Andel Institute
- Managed by puppet, deployment with foreman

Presentation from HEP sites on Dynafed:
- <u>Dynafed is redirector for dynamic data federation</u>, client accessing data is redirected to closest storage element (dCache, Ceph and S3-compatible)
- In testing by Atlas (RUCIO) and Belle-II sites in US. <u>Benchmarked their distributed storage endpoints with distributed geographically clouds (grid), confident of replacing on-disk Grid SE with Dynafed,</u> build extensive monitoring for Dynafed

Storage and Filesystems
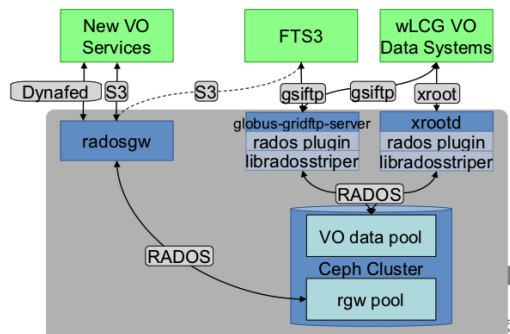## Site infrastructure developments and updates

Presentation from Vanderbild Uni on LStore HDFS Integration:
- Presented cost-effective replacement for GPFS with LStore and HDFS:
  lstore:// connector via org.apache.hadoop.fs.FileSystem.LStoreFileSystem
- LStore is generic block level storage abstraction for HPC multi-user
  environment, integration of HDFS boosts read effectiveness
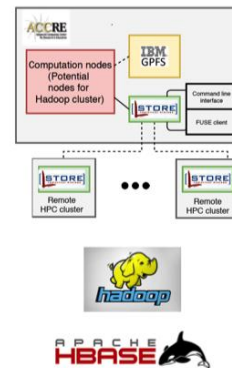
Presentation from UK RAL (Tier 1) on ECHO:
- Presented ECHO disk storage - erasure-encoded high-throughput object
  store. CEPH based object storage, access via GridFTP/XRootD/S3. Goal
  of ECHO is maximising throughput. Random-access for their use-case no
  important. All data in erasure code, no replication used (even for hot data)
- Improvements for CASTOR (minimised configuration complexity)

Storage and Filesystems

Site infrastructure developments and updates

Presentation from Karlsruhe Institute of Technology (Tier 1) on use of virtualized storage cluster
- Virtualization cluster using oVirt / RHV with KVM hypervisors. Hyperconverged setup with Gluster storage.
- Server VMs are "close to storage" in hyperconverged
- Tests with HPC access to storage cluster
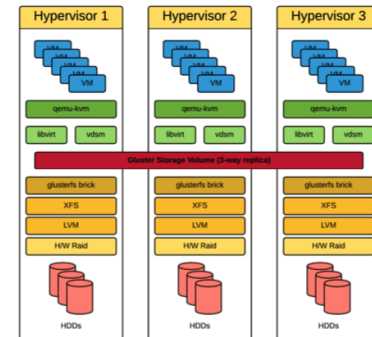
Presentation from Brookhaven Laboratory on their storage management practices
- Brookhaven presented how their manage their JBOD storage racks (they showcased scripting they use)

Presentation from CERN on storage services:
- Update on status of storage services (EOS, Castor, AFS, Swan, CERNBox, Ceph, CVMFS)
- Plans to phase out AFS has been delayed but still on target for completion before run 3. Announced to sites using the AFS the disconnection test
- Presented the FuseX, new namespace architecture with QuarkDB, Migration to EOSHOME and CERNBox as App Hub with SWAN, Office Suites etc
- Presented evolution of CEPH (2nd region for s3, demand as backup-storage, CVMFS backend phase-out to s3)

Grid, Cloud and Virtualization (1)

Addressing the Challenges of Executing Massive Computational Clusters in the Cloud
Boyd Wilson (Omnibond)

- Omnibond Automaton / PAW tool to create, scale, use and destroy a cluster in commercial cloud environments
- CCQ: meta-scheduler over several clusters
- Two examples were presented:
  - Using CloudyCluster to spawn a cluster of 1.2 million cores on AWS in less than two hours; increased (~ x2) the public price of compute resources in AWS' US regions
  - Using traffic video data with AI algorithms for accident detection, congestion analytics and improve traffic flow

CloudScheduler version 2
Rolf Seuster (University of Victoria)

- CloudScheduler starts VMs which run HTCondor when they boot
  - Currently compatible with OpenStack, AWS next
- Rewrite of CloudScheduler v1 released in 2009
  - Python 3 and MariaDB
  - The CLI and the GUI call the same REST endpoints
- In production in ATLAS since several months; in Belle II next

Grid, Cloud and Virtualization (2)

The GlideinWMS system: recent developments
Marco Mascheroni (UCSD)

- GlideinWMS looks at user jobs in the Condor schedulers
  - Matches them to Computing Elements
  - Determines the number of pilot jobs to submit via Glidein factories
- Supports EC2 and GCE
- New features have been introduced
  - Singularity support
  - Whole-node allocations

The Experience and Challenge in Grid Computing at KEK
Go Iwai (KEK)

- KEKCC:
  - 10k CPU cores, 2TB memory, Linux cluster and storage system
  - Replaced every 4-5 years
  - Mostly running Belle II workloads now
- Data migration from Belle to Belle II
  - 1PB, 15M files
  - Estimated 2 months, took one year (busy system, software issues)
- Massive Data Transfer performance issues
  - Some workarounds found thanks to efforts from both KEKCC and Belle II
  - Highly anticipated KEKCC upgrade in 2020

Grid, Cloud and Virtualization (3)

Creating an opportunistic OSG site inside the PRP Kubernetes cluster
Igor Sfiligoi (UCSD)

- Pacific Research Platform
  - Kubernetes cluster of 2.5k CPU cores, 250 GPUs
  - Nautilus web interface for self-service
  - Mostly ML/AI use cases
  - Little contention: happy users, but GPUs underutilized
- Opportunistic jobs for OSG users
  - Mostly from the IceCube community
  - One worker node per available GPU
  - Pod priority very low to allow preemption; HTCondor supports it
- Container-Storage-Interface (CSI) to mount CVMFS in the containers
  - Work In Progress in liaison with CERN
- Native OSG support for Kubernetes is desirable to reduce the amount of glue code

Grid, Cloud and Virtualization (4)

Public cloud for high throughput computing
Dr Gregory Parker (Entonos)

- Compute-intensive simulations of modern hard drive techniques (heat assisted magnetic recording - HAMR)
- Leveraged AWS Spot (preemptible) instances and S3 for storage
- Fleets of 100k concurrent simulations achieved with 99,99% of the cost just for compute
  - Eventually scaled out to a million without modifying the abstraction layer
- Cloud surprises: variations in compute performance, S3 latency at scale

6 years of CERN Cloud - From 0 to 300k cores
Belmiro Moreira (CERN)
- LxCloud, CVI, OpenStack
  - From 2 to 70+ cells; upgraded to CellsV2
  - Storage: Cinder, Manila, S3
  - Deprecation of Ceilometer, as it was hard to maintain
- In 2019
  - 2 cloud regions: Batch vs. Personal / Services
  - Preemptible instances
  - OpenStack control plane in container clusters
  - nova-network ➔ Neutron migration, SDN
  - Enrolling of hypervisors in Ironic

Grid, Cloud and Virtualization (5)

Developing for a Services Layer At The Edge (SLATE)
Ben Kulbertis (University of Utah)

- SLATE: Kubernetes-based distributed service orchestration platform
- Developers deploy services based on Application Catalogs (Helm charts)
  - Can be contributed to a Git repository via a merge request
- Developer environment:
  - Minikube considered, but it has limitations and overhead
  - MiniSLATE: local, dind one-node SLATE setup

Changes to OSG and how they affect US WLCG sites
Jeffrey Michael Dost (UCSD)

- Spring 2018: OSG transitioned to Indiana University
- OSG CA discontinued; sites should use Let's Encrypt or IGTF InCommon
- OIM transitionned to OSG Topology (catalog of all OSG sites stored on GitHub)
- Hosted CE: OSG-managed compute elements that just require remote SSH login
- OASIS (CVMFS repository), StashCache (XRootD federation for VOs), OSG Glidein factory…

IT Facilities and Business Continuity (1)

Cost and system performance modelling in WLCG and HSF: an update
Jose Felix Molina (CIEMAT), Dr Andrea Sciabà (CERN)

- Gap between available resources and expected needs for HL-LHC
  - 10x increase in trigger rates, 5x increase in pile-up
  - CPU and disk short by a factor of 2
- The WG identified some reference workloads for each experiment
  - Having a common framework for modelling the computing requirements turns out to be unrealistic
  - A spreadsheet implements a model for calculating TCOs and budget; discussions ongoing to reach an approach usable by all sites

RACF/SDCC Datacenter Transformation
Alexandr Zaytsev (BNL)

- Moving from their 1.5MW air-cooled datacenter to a new building (former Light Source)
  - Fully power redudant
  - Water-cooled racks
- Construction will start in April 2019; move expected to be completed by FY23
- 1.6Tbps between the two data centers
- No service interruption foreseen

IT Facilities and Business Continuity (2)

Omni, N9 and the Superfacility
Cary Whitney (LBNL)

- Perlmutter (2020): new Cray system providing 3-4x the performance of the existing Cori installation
- Leverages Cray's Slingshot networking: 3 hops max between any node, ethernet compatible
- All-flash filesystem: 30PB, 4Tbps bandwith, 7 000 000 IOPS
- Support for containers and Python-based analytics with GPUs
- 12MW upgrade to the facility required

HEPiX Technology Watch working group
Helge Meinhard (CERN)

- Created in Spring 2018; 58 subscribers to the ML
- Organized in six sub-groups:
  - General market trends
  - CPUs and accelerators
  - Servers
  - Memory
  - Storage
  - Network
- Server costs: CPU and storage price/performance thought to be improving by 15% and 20% per year; ultimately found to be lower than that. WG participants should find a way to gather some data to better understand the trends

IT Facilities and Business Continuity (3)

Network TechWatch report
Rolf Seuster (University of Victoria)

- Internet traffic is expected to increase by a factor of 3 between 2017 and 2022
- Ethernet evolutions
  - P802.3cn: 50/200/400Gbps over single-mode fiber
  - P802.3cp: bidi 10/25/50 Gbps for the Access
  - P802.3ct: 100/400Gbps over DWDM
- PAM4 and FEC to drive higher speeds and port density
- 100 Gbps server interfaces introduced at SC18

Server TechWatch report
Michele Michelotto (Università e INFN, Padova), Martin Gasthuber (DESY)

- Data centers use ~3% of the world's electricity out, could reach 20% in 2025
- 42U rack can draw around 40kW; watercooling becomes more and more popular, but there are concerns about the power consumptions
- Open19: new open-source platform for servers
  - Rack, cage or network switch
  - 4 form factors for servers
  - Allegedly more economical compared to Facebook's OCP
- Open Computing Platform: new Open Rack v2, Server or Drive Tray

IT Facilities and Business Continuity (4)

Storage TechWatch report
Andrea Chierici (INFN-CNAF)

- Hard Drive Disks
    - IOPS per TB continue to fall: dual actuator coming in 2019
    - Reaching the density limit for perpendicular magnetic recording: MAMR & HAMR should allow 40TB drives by 2025
    - Concerns about the shrinking market; narrowing price with SSDs
- Solid State Drives: expanding beyond SATA
    - NVMe eliminates some software layers in the OS stack; it's the center of industry attention
    - NVDIMM: persistent memory, DDR4 / DDR5 form factors (CPU support required)
- Tape: still key technology for large-scale archival
    - LTO: Gen-8 released in Q4 2017-360MB/s, 12TB
    - Concerns about the shrinking competition on both drives and media

End-user IT Services and Operating Systems (1)

- **Text Classification via Supervised Machine Learning for an Issue Tracking System**
  Martin Kandes (UCSD)

  - HPC User Services Group: handles end-user support tickets
  - Goals:
    - Classify incoming user tickets
    - Provide generic but useful automated replies as a first level of support
  - Several models experimented: naive / scikit Bayes classifier, TensorFlow...
    - Scikit MLP showing the best accuracy
  - Results promising
    - 0.5 to 0.95 accuracy, depending on the topic
    - Plans to explore more completely some ML approaches, such as multilayer perception (MLP) and Support Vector Machine (SVM) more completely
    - XOAuth2 support with Outlook Mail API in the pipeline

End-user IT Services and Operating Systems (2)

Endpoint user device and app provisioning models
Michal Kwiatek (CERN)

- Goal: to understand endpoint user device landscape at CERN
- Data collection: anonymized SSO / email logs, user survey
  - 57% of users who access CERN e-mail use CMF
  - 26% of users who access CERN e-mail use also Self-Service
  - 5000 Android users, 4000 iOS users
- Strategy: focus on application management rather than device
  - Offer apps repositories for all platforms
  - Provision licences

How to make your Cluster look like a Supercomputer (for Fun and Profit)
Georg Rath (LBNL)

- SMWFlow: Git-based management tool to manage system states, developed in partnership with Cray
  - Code reviews, testing, reproducibility
- Added a SMW layer on top of all systems for them to be manageable by SMWFlow
- Custom management stack built on top of xCAT and cfengine

Site Reports

NERSC/PDSF
- Migration to Cori (Cray XC40, 12.076 nodes, 700k cores) for workloads complete
- PDSF computing cluster turned off

University of Nebraska CMS Tier2
- Extending useful lifetime of equipment to stretch resource availability

BNL
- New data center - beginning of construction in April 2019
- Migrated from OpenLDAP to RedHat IPA
- Transitioning from Shibboleth to Keycloak for service auth
- Jupyter service has been re-architected with a unified environment on Red Hat Enterprise Virtualization cluster

Site Reports

Canadian T1 / T2
- all T1 services previously at TRIUMF moved to SFU (~30km or 1ms RTT away)
- new T2s in Canada at UVic, SFU, Waterloo, ETS (T3 facility, might be upgraded to T2)

AGLT2 – ATLAS Great Lakes Tier 2
- Significant work to improve the utilization of the cluster (increase CPU utilization rate)
- Reconfigure low memory nodes, making all the cores being claimable by HTCondor

University of Wisconsin-Madison CMS T2
- Using opportunistic resources at CHTC for CMS production jobs (average of ~1.5k cores used)
- Deployed XrootD over HTTPS and upgraded cluster from Scientific Linux 6 to CentOS 7.6

Site Reports

KEK
- Ramp-up in resource utilization due to Belle-II and J-PARC physics data
- The renewal of KEK campus network was completed in September 2018

Tokyo Tier-2 - International Center for Elementary Particle Physic
- Hardware in the computing center supplied by a lease, replaced every 3 years
- Completed migration to new hardware as a new system was delivered in Jan 2019
- all Grid services and worker nodes are running on CentOS 7

FNAL
- Moving service certs to InCommon CA after OSG CA shut down last year
- HEPCloud now live (scientific gateway to resources beyond local worker nodes and grids, expanding HPC centers and the cloud)

Site Reports

UW CENPA

- Repurposed previous generation of PDSF hardware donated by NERSC to upgrade their existing cluster

JLab

- New GPU cluster installation is underway (32 servers, each with 8 RTX 2080 GPUs)
- Increase offsite resource usage at NERSC, OSG, and also in the cloud

IHEP / BEIJING-LCG2

- Became LHCbTier 2 site
- Significant improvements to their monitoring and fault analysis platform

Site Reports

INFN

- Infrastructure work still on-going as part of plan to address previous data center flooding
- Next-Generation Firewall installed(Palo Alto PA-5250)
- 2 racks now implement an ISMS (CNAF got ISO27001 certification in 2017)
- Several scientific collaborations interested in hosting medical data there

NIKHEF

- More systems now configured with Salt (LDAP, DNS, dCache)
- Migrated from Nagios to Icinga2
- Working on setting up a high-throughput private compute cloud with Openstack

Site Reports

RAL

- SCD cloud delivers dynamic compute resources to scientists across STFC and externally (IaaS platform built on OpenStack)
- New tape cache pool running CASTOR version 2.1.17-35
- Decommissioned "disk-only" CASTOR pools in favour of Ceph-based storage

DESY

- Jupyter Notebooks very well received (especially by Photon Science users)
- Migration to Windows 10 - no DESY accounts or information in Microsoft Clouds
- Large fully featured MS Windows 10 roll-out (now 40:60% ratio for Win10 vs Win7 usage)
- Storage options considered for the future
  - replace OpenAFS with AuristorFS ? (tests underway)
  - going Sync&Share only? (based on NextCloud and dCache)

Site Reports

FZU / Prague
- New cluster based on HPE Apollo 35 (AMD EPYC 7301 CPU)
- Network upgrade - Catalyst 6509 and Nexus 3172 switches replaced with Catalyst 9500

GSI
- GDPR: several inquiries requesting access to personal data (challenging for IT)
- Windows 7 to 10 migration in progress

Diamond Light Source
- New scientific data processing cluster (2.560 Xeon Gold 6148 cores, 8PB GPFS 5)
- Making use of on-premise or STFC OpenStack cloud resources

Basic IT Services

Configuration Management and Deployment Setup at KIT
- many different approaches including Ansible, KITE (homegrown system) and Katello/Satellite/Foreman + Puppet
- Foreman/Katello manage all aspects of host life cycle
- Next steps: migration to Puppet 6

Token Renewal Service at SLAC
- Need to upgrade its token renewal service – used since the late 1990s
- Many options available: kcron, k5cron, etc.
- Work in progress

Network & Security

BNL activities on federated access and Single Sign-On

- Why: several Kerberos realms, Shibboleth config/mgmt is complex, SSO and Federated access wanted
- Based on RedHat Identity Management (easy install and setup, redundancy with with multi-master replication and read-only replicas)
- Migrated users from OpenLDAP to IPA
- Keycloak deals with authentication (2F auth easy to setup)

- Status:
  - Invenio test prototype now has federated access
  - Jupyter test instance has MFA access enabled using KeycloakQR codes
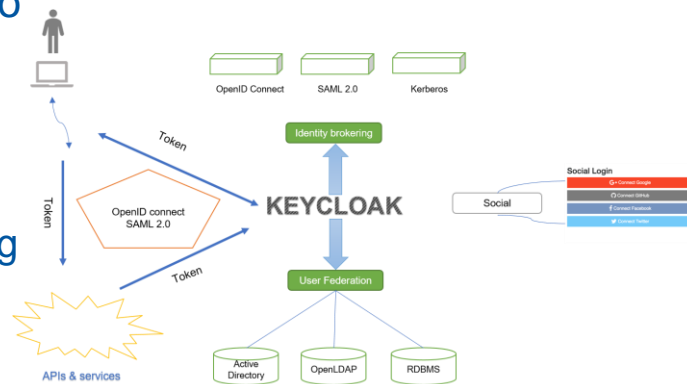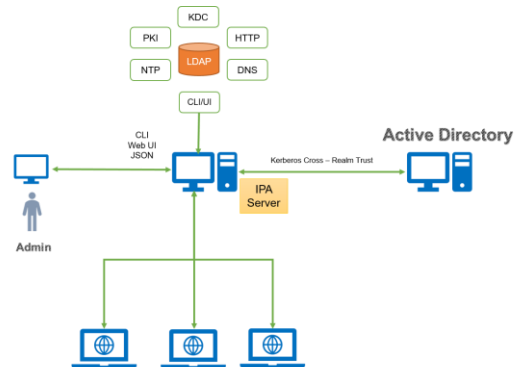
Network & Security

Situational Awareness: Computer Security

- Data leaks, CPU vulnerabilities, crypto mining
- Credential exposed, software licences, etc.

DNS and DHCP service evolution plans @ CERN

- Rewrite DNS-related software in Go
- Use the ISC Kea DHCP server (database back-end, working HA, REST API)

Network & Security

Differences in network equipment and how to break them

- Same chips in products from different vendors but differences in software stack, CLI, support, etc.
- Performance and scaling tests on selected network equipment

IPv6 & WLCG – updates from the HEPiX IPv6 WG

- All T1 sites connected to LHCONE except RRC-KI
- TRIUMF, CERN, KISTI and RRC-KI still have some problem with IPv6 on perfSonar
- Tier-1s should already have production storage accessible over IPv6 (more than 85% of data is available via IPv6)
- 37% of FTS transfers today over IPv6

Network & Security

WLCG/OSG Network Activities, Status and Plans
- perfSONAR – 261 active instances
  - new plugins: network traffic capture and TWAMP (two-way active measurement protocol)
  - new central web interface and toolkit configuration mechanism
- 'New' Collaborating Projects: IRIS-HEP and SAND (coordinates network monitoring and diagnostics)

HEPiX Network Functions Virtualisation WG Update
- Role: evaluate whether and how SDN and NFV should be deployed in HEP
- Wide range of SDN solutions for data centres exists
- Focus on Open vSwitch/Open Virtual Networking and Tungsten Fabric (both open source)
- SmartNIC now offered from multiple vendors
- SENSE and BigData Express leading projects in programmable networks
- Initial report/white paper - in progress

HEPiX Fall / Autumn 2019
14 - 18 October, Amsterdam

Nikhef

Photo by Raphael Nogueira on Unsplash

Next meetings

NIKHEF
Amsterdam, The Netherlands
14 - 18 October 2019

ASGC
Taipei, Taiwan
Spring 2020

Fall / Autumn 2019
14 - 18 October, Amsterdam

HEPiX

Nikhef