

# Unix Town Hall Scientific Computing S

Scientific Computing Services

August 27th, 2020







### **Unix Town Hall Meeting**



### Objectives:

- Communication
- Collaboration

Join our mailing list: unix-community@slac.stanford.edu

email to: <u>listserv@slac.stanford.edu</u>

subscribe unix-community

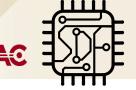
### **Scientific Computing Services**



unix-admin@slac.stanford.edu support/questions

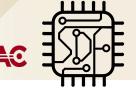
yemi@slac.stanford.edu 650-926-2863

### **Scientific Computing Services**



- New production version of Confluence is coming in September
- Available for testing today: <a href="https://confluence-uat.slac.stanford.edu/">https://confluence-uat.slac.stanford.edu/</a>

### **Scientific Computing Services**

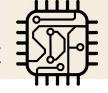


### **WE ARE HIRING!!**

**Job #4118: High Performance Computing Administrator - UNIX Clusters** 

**Job #3970: Unix Scientific Computing Specialist** 

### **Unix Town Hall Meeting**



### Agenda:

- Welcome our new CIO Jon Russell
- Partnership & Engagement: 12-month recap (Yemi)
- SDF Beta Environment (Yemi)
- Active Directory accounts for Identity Management (Karl)
- SDF User Experience (Yee)
- NERSC (Debbie)
- Intermission
- SDF Filesystem Update (Lance)
- Batch Compute Update (Yemi)
- Tape Storage Roadmap (Guangwei)
- Storage Update (Lance)
- CentOS / RHEL Platform Update (Karl)
- Next Steps for SDF (Yemi)
- Cyber Security (Olga)
- Questions/Discussion



# Jon Russell SLAC CIO







### A little about me...

- 20+ years experience in IT
- 6 Years in Stanford University IT
- 10 Years with the DOD
- 2<sup>nd</sup> Time as a CIO



### **SLAC IT Focus Areas**



|                | Improve the Customer Experience          |
|----------------|--|
|                | Connect to the Research Mission          |
| <b>■</b>       | Improve Communication & Transparency     |
| In the second  | Build Strength through Partnerships      |
| O <sub>0</sub> | Modernize Infrastructure & Core Services |



### **Issues of Potential Interest**

- Improving the level of communication
- Identity and Access Management (IAM) Roadmap
- Operationalize Shared Data Facility (SDF)
- SRCF-II
- DOE GCP Contract
- Unix Account CS100 Requirement





# Partnership & Engagement: 12-month recap

Yemi Adesanya

August 27th 2020, Unix Town Hall







### Partnership & Engagement: 12 month recap



#### Q4 FY19

- SDF core networking and storage components jointly funded by LCLS and SLAC IT
- Machine Learning funds GPU cluster (~\$250K) along with additional storage capacity and performance (~\$240K)

### Q1 FY20

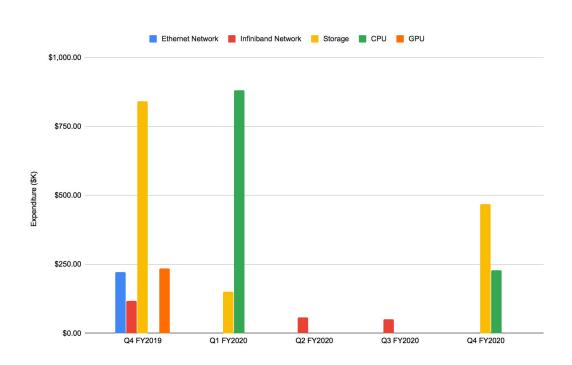
- CryoEM purchase drive capacity
- 11264-core AMD "Rome" CPU cluster purchase with funding from LCLS, HEP (Fermi, HPS, SuperCDMS), CryoEM, SUNCAT (BES)

#### Q2,Q3 FY20

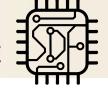
- B050 Datacenter deployment with further investment from HEP and SUNCAT to complete the SDF networks
  - Jointly funded by LCLS, Machine Learning, SLAC IT.
  - Special thanks to Networking and Datacenter
     Teams for working under challenging social
     distancing conditions

#### Q4 FY20

- Another major storage expansion purchase funded by ATLAS, CryoEM, KIPAC, SLAC IT
- Additional 2560 AMD cores for KIPAC

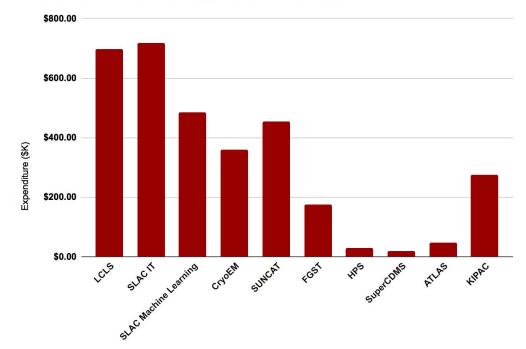


### Partnership & Engagement: 12 month recap



- SLAC has committed more than \$3.2M committed to SDF network,storage and compute since Q4 FY19
- SDF = "Shared"SDF != "Siloed"
- A single, integrated facility for data analytics
- Maximize utilization by leveraging idle cycles (opportunistic)
- Multi-tenant filesystems with scalable capacity and performance
- Drive for a sustainable Baseline with continual support and funding from SLAC IT (indirect).

### SDF Infrastructure Investment since Q4 FY20





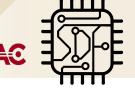
Yemi Adesanya

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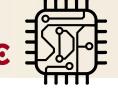








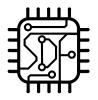
- SDF is online, but we're not ready to declare full production status
- Beta testing group of users have started building analysis environments and submitting jobs
- Ongoing Datacenter work
  - Network, power distribution and load-testing
- Filesystems are mounted and DDN we've been performance tuning
  - Distributed Namespace, Data-on-Metadata, Progressive File Layout
- Wanted: users who can withstand some rapid changes and provide feedback
  - Be prepared for unscheduled outages and configuration changes
- Why does SDF initially appear somewhat bare-bones?
  - This really is our attempt at a new compute facility for SLAC
  - The goal is to minimize dependencies on the existing Unix services
  - Add packages and services to the software stack "as needed" rather than pull in "everything" by default



- "/sdf" is the primary filesystem
  - All home directories under "/sdf/home/"
  - Shared project/group directories under "/sdf/group/"
  - Lustre project quotas applied to subdirectories
- Limited number of GPFS filesystems available
  - StaaS, Fermi, CryoEM
- No SLAC Automount map
  - The goal is eventual migration to native SDF storage
  - Contact unix-admin if you need help moving data to SDF
- "/sdf" is mounted on a select number of existing non-SDF systems
  - centos7\*, rhel6-64\*, bullet\*, bubble\*, kiso\*, deft\*
  - Helping users transition existing workloads to SDF compute environment
- Environment Modules interface for selecting installed software packages <a href="https://en.wikipedia.org/wiki/Environment Modules">https://en.wikipedia.org/wiki/Environment Modules</a> (software)
  - o OpenMPI, FFTW, HDF5, etc
  - Provide access to the latest releases in the Red Hat Software Collections distro
- SDF Beta is now open to everyone. There are no login restrictions. We welcome your input



### Questions?



# Active Directory accounts for Identity Management

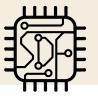
Karl Amrhein

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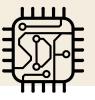


### Active Directory accounts for Identity Management



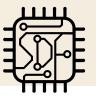
- For our discussion today, what is "Active Directory", also known as, "AD"?
  - It is a Kerberos authentication server (username and password, is account disabled?, etc.)
  - It is an LDAP server (linux openIdap tools can be used for queries, same way you query Unix LDAP).
    - An example of something stored in LDAP is: Unix POSIX groups (primary and supplementary).
- Why are we doing this?
  - Reduce duplication of effort do we really need Kerberos and LDAP servers on Unix and Windows?
    - Managing parallel infrastructures for Kerberos and LDAP is expensive and time consuming, and this critical infrastructure takes extra special effort manage securely. "keys to the kingdom"
  - Moving towards a single SLAC Identity (AD) means one less account to manage; one less password.
    - Identity and Access Management (IAM) project goals include improved single sign on. Using a single account (AD, or "SLAC ID") for authentication and authorization moves us in that direction.
  - SDF "greenfield" is a unique opportunity to modernize our authentication and authorization, and make some transformational changes. Using AD for authentication is a common, modern practice documented by Red Hat, and other Linux distributions.
    - https://access.redhat.com/documentation/en-us/red\_hat\_enterprise\_linux/7/html/windows\_integration\_guide/
    - https://sssd.io/docs/users/ad\_provider.html

### Active Directory accounts for Identity Management



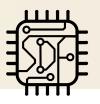
- How does this actually work?
  - ssh to sdf-login01 or sdf-login02. Enter your SLAC username as always, but your Windows password.
  - Kerberos works the same as you might be used to:
    - type "klist" and you will see a Kerberos Ticket Granting Ticket (TGT).
    - except you'll see it say "<u>username@WIN.SLAC.STANFORD.EDU</u>" (note the "WIN")
    - "kinit -R" will renew your TGT before it expires, without typing a password.
  - Your username, UID, and GIDs are the same inside SDF as outside SDF (eg, rhel6-64, centos7)
    - Your AD account object includes two attributes which allow linux login: uidNumber and gidNumber
    - on sdf-login01 or 02, type "id" or "id [username]" to see your UID and GIDs, or someone else's
    - Configuration on linux host for database lookup order: /etc/nsswitch.conf -> SSSD -> AD
    - standard commands such as "getent" still work (display entries from databases in nsswitch.conf)
      - eg, "getent password [username1 username2 ...]", or "getent group [group1 group2 ...]"
  - openIdap client tools can be used to query Active Directory. openIdap command lines are unwieldy, so we have provided a couple of scripts on sdf-login01 and 02 which can list all usernames and all POSIX groups defined on the system: "listusers [username1 uid2 ...]", "listgroups [groupname1 gid2 ...]", "listusers" (to view all users), "listgroups" (to view all groups).

# Active Directory accounts for Identity Management SLAC



- What is not changing:
  - usernames and UIDs, group names and GIDs
    - we are keeping the legacy group names and GIDs to ease storage migration and keep the same access to it (eg, existing file and group ownership and permissions work in SDF)
  - the management of unix groups is not changing: use 'ypgroup' (for now) on rhel6-64.
    - the larger Identity and Access Management (IAM) project will modernize this process
- What if a SLAC user has a unix account but does not yet have an Windows/AD account?
  - o self-service web portal to create an AD account for SDF login access, if you already have unix account
    - https://ad-account.slac.stanford.edu

# Active Directory accounts for Identity Management SLAC



### Questions?



# **SDF User Experience**

Yee-Ting Li

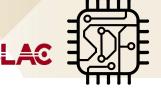
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### General



- compilers etc.
  - gcc still generally recommended, newer versions (7+) will be provided
  - intel to be added
- openmpi 4.0.4 as standard
- modulefiles as standard now
  - free to continue to install software as is; but it does...
    - provide a layer of portability (just modify modulefile instead of changing hard coded paths)
    - visibility for other users who may also want to run same software
  - build your software in docker/singularity containers
    - allows portability and better application management
    - wrap a modulefile around it!
- will have examples in documentation site...

### **Better Documentation!**

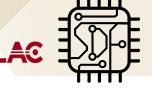
### Previously:

- numerous (and old) documentation around
- groups would often write their own documentation
- pages are on html files or restricted write confluence pages/other wiki
- not searchable in google etc.
- status and performance information fragmented and difficult to customise

### Goal:

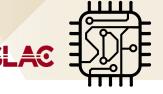
- provide easy to maintain, community driven documentation on everything SDF
- User guides, tips, FAQs etc.
- Easy for anyone to contribute (both inside SLAC and outside)
- Reduce the duplication and redundancy of information
- Put somewhere where people can find and read it!

### Web based tools for SDF



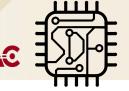
- https://jupyter.slac.stanford.edu will be deprecated
  - jupyterhub (at least the way its been implemented) doesn't meet the needs of scalable, integrated and reliable infrastructure.
  - pros:
    - simple interface
    - (convoluted) bring your own jupyter
  - cons:
    - use of docker containers for runtime meant integration had to be reviewed for cyber security reasons
    - limited resources: wasn't integrated into slurm, so separate k8s nodes were required
- web-based access
  - integrate monitoring; easily check up status
  - file upload/downloads

### **Single Frontend**



- In development currently (lots left to write)
  - https://ondemand-dev.slac.stanford.edu
- backed with github and markdown files
  - users can submit changes through github and we can review with 'pull-requests' to merge changes
- will be moved to <a href="http://sdf.slac.stanford.edu">http://sdf.slac.stanford.edu</a>

### **Demo**



https://ondemand-dev.slac.stanford.edu

### **SDF User Experience**



### Questions?



# **NERSC Update**

Debbie Bard August 27th 2020, Unix Town Hall









### Intermission



# **SDF Filesystem Update**

Lance Nakata

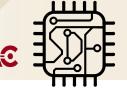
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### **SDF Filesystem Update**



- Two DDN ES18KE subsystems, fully redundant
- Internal SAS SSDs for metadata targets (MDTs)
- 10 external disk trays, ~7.3PB /sdf, ~24TB /scratch
- Plan to add 10 more disk trays during Q1FY21 and perhaps double /sdf capacity
- Runs DDN's EXA5 software, based on Lustre 2.12.3 with DDN extensions
- Disks use Declustered RAID (DCR) software for protection and faster rebuilds

### SDF Filesystem Update (cont'd)



- Distributed NamespacE Phase 2 (DNE2): distribute a directory's contents over multiple MDTs. Used for directories with (potentially) large subdirs within them
- Data on MDT (DoM): write first 1MB to MDT for better small file I/O performance
- Progressive File Layout (PFL): automatically adjust striping policy based on filesize
- Block and inode quotas on all directories (mostly based on projectIDs)
- Default home directory quota: 25GB and 500K inodes

### **SDF Filesystem Update**



### Questions?



### **Batch Compute Update**

Yemi Adesanya

August 27th 2020, Unix Town Hall







#### **Batch Compute Update**

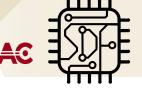


#### Rome CPU Cluster

- AMD Rome EPYC 7702 CPUs @ 2.0GHz
- 4GB RAM per core
- 100Gb Infiniband
- 11264 total cores or 176 TFLOPs
- Currently fully-funded via science directs
- 5-year hardware lifecycle
- Partially deployed as of 8/2020
- Datacenter is working hard to resolve B050 power distribution challenges
- \*Additional 2560 cores coming for KIPAC

| Project   | # Cores |
|-----------|---------|
| LCLS      | 2816    |
| Fermi     | 2048    |
| SUNCAT    | 5376    |
| CryoEM    | 384     |
| HPS       | 384     |
| SuperCDMS | 256     |
| KIPAC*    | 2560    |

#### **Batch Compute Update**



- Access via slurm job scheduler
  - We have a developer support agreement for the SDF CPU & GPU clusters
- We must ensure paying stakeholders get instant access to their dedicated partition
  - Delegate an owner (POC) for each partition that can manage their group membership
- A shared queue is available for opportunistic job submissions
  - Run the risk of preemption (job termination)
  - Recommend checkpointing your code
  - Can we justify indirected funded cores? How many?
- TO DO: Generate periodic utilization reports (monthly or quarterly) for each partition
  - Help stakeholders plan for lifecycle and support their grant proposals

## **Batch Compute Update**





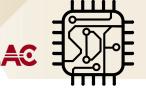
# **Tape Storage Roadmap**

Guangwei Che August 27th 2020, Unix Town Hall





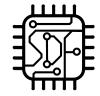
## **Tape Storage Roadmap**



- We currently own two Oracle SL8500 tape libraries
- Oracle stopped enterprise tape drive development in 2017. Growing concern about
   Oracle's tape commitment plus increasing library maintenance and media costs
- Potential tape library replacements: IBM TS4500 and Spectra Logic TFinity
- Uncompressed tape library capacity of 120-160 PB, expandable to over 1 EB via media frame additions and drive upgrades
- Tape drive choices: TS1160 (20TB) or LTO-9 (18TB)
- Upgrading tape drive technology to enhance data migration rate to 6 GB/s or above
- Exploring solutions to archive SDF cold data to tape to reduce disk storage expense
- Planned tape library deployment: FY21

## **Tape Storage Roadmap**





# **Storage Update**

Lance Nakata

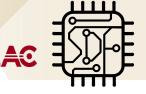
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### **Storage Update**



- Storage as a Service (StaaS)
  - StaaS disk hardware is 90% full and entering retirement
  - No additional space planned for this service
  - Will be transitioning experiments to SDF storage starting FY21
- Hardware Lifecycle
  - FY21 and beyond: retire legacy Sun, LSI, and Dell storage
  - Groups can migrate data to SDF storage, delete it, or archive it to tape (additional cost)
  - You will receive migration (downtime) notices for data moves





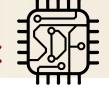
Karl Amrhein

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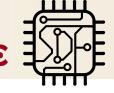








- Red Hat Enterprise Linux Life Cycle: <a href="https://access.redhat.com/support/policy/updates/errata">https://access.redhat.com/support/policy/updates/errata</a>
- Red Hat Enterprise Linux 5
  - Extended Lifecycle Support (ELS) ends November 30, 2020
  - No updates at all after that date.
- Red Hat Enterprise Linux 6
  - "Maintenance Support 2" ends November 30, 2020
  - Extended Lifecycle Support (ELS) starts after that.
- Recommended Operating System / Linux Distribution
  - For servers: CentOS 7 or RHEL 7
  - For desktops/laptops: Ubuntu LTS (recommended) or CentOS 7
- Support for CentOS 8 coming next year, after RHEL 5 systems have been retired



- Configuration Management
  - Taylor for RHEL 5 and RHEL 6
  - Chef for CentOS 7, RHEL 7, Ubuntu LTS
- SLAC Chef cookbooks (configuration management code) on github:
  - https://github.com/SLAC-CHEF/
  - Send your github username to unix-admin and we will add you to the SLAC-CHEF organization
    - Then you can request/recommend code changes
- Unix Platform work in progress
  - Support of SDF, especially regarding changes to authentication
  - Support of IAM project and integration of the InCommon Trusted Access Platform suite
    - https://spaces.at.internet2.edu/display/ITAP/InCommon+Trusted+Access+Platform+Library
  - Remaining RHEL 5 servers need to be replaced with CentOS 7 or RHEL 7, so we can focus on RHEL 8
  - Retire OpenStack cluster: migration to VMware or Containers instead





# **Next Steps for SDF**

Yemi Adesanya

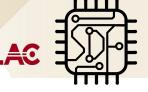
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#### **Next Steps for SDF**



- Short-Term
  - Comprehensive user guide for SDF on the github site
  - Complete the CPU cluster deployment in B050 datacenter
  - Begin migration of all GPU nodes into SDF
  - Establish the base compute software stack via Environment Modules interface
  - Complete the recently purchased storage expansion includes capacity for CryoEM, ATLAS and KIPAC
  - New Tape Library (Phase 1)
  - Assemble a steering group to review our current/proposed SDF operational policies and usage quotas
- Longer-Term
  - Datacenter strategy to support SDF growth beyond B050 (SRCF-II,.....)
  - Cost model and budget projections for Computing (indirect) funding to deliver baseline SDF capabilities
  - Align to SLAC IAM roadmap and consider Federated Identity models
  - Facilitate NERSC for SLAC computing
  - Opportunity for SDF cloud Proof Of Concept