# Customizing RUCIO at LCLS

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SLAC NATIONAL ACCELERATOR LABORATORY

# LCLS - Linac Coherent Light Source

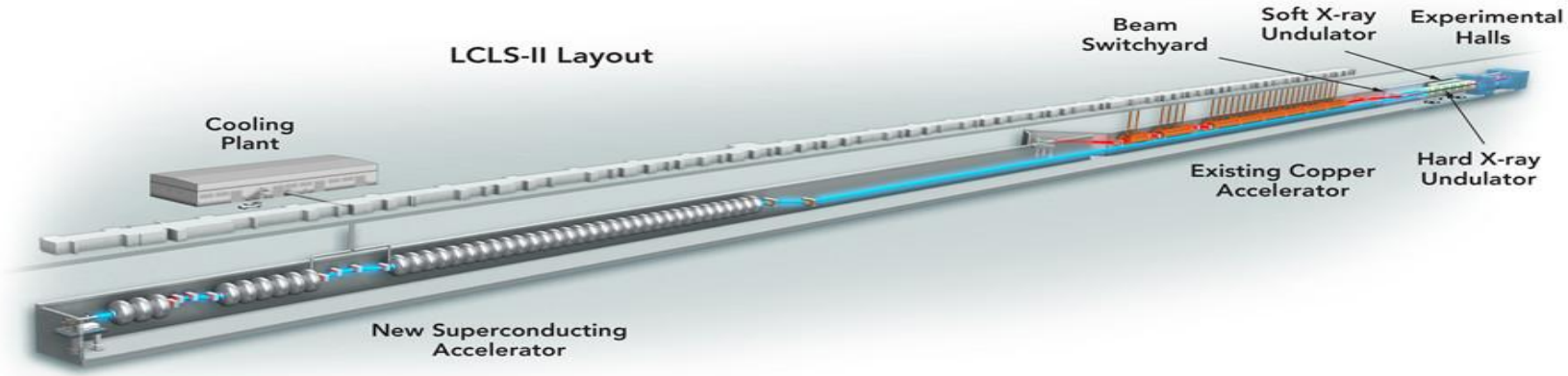
**The LCLS is a free electron laser that produces ultra fast X-ray pulses.**

**LCLS has already had a significant impact on many areas of science, including:**

- ➔ Resolving the structures of macromolecular protein complexes that were previously inaccessible
- ➔ Capturing bond formation in the elusive transition-state of a chemical reaction
- ➔ Revealing the behavior of atoms and molecules in the presence of strong fields
- ➔ Probing extreme states of matter
- ➔ Covid-19 research, e.g. imaging of SAR-CoV2 spike protein

# LCLS-II

- LCLS has been operating since 2009 using SLAC's warm copper linear accelerator
- LCLS has provided a wide spectrum of exiting scientific results
- For LCLS-II a new superconducting accelerator is being build and the science program is scheduled for 2022
- LCLS-II will provide a jump in capabilities allowing experiments that were not possible so far.
- The pulse rate will jump to about 1MHz from the current 120Hz of the copper linac.
- Data rates will jump from a few GB/s to TB/s  (data written out will be smaller)
- Both accelerators will be operated in parallel

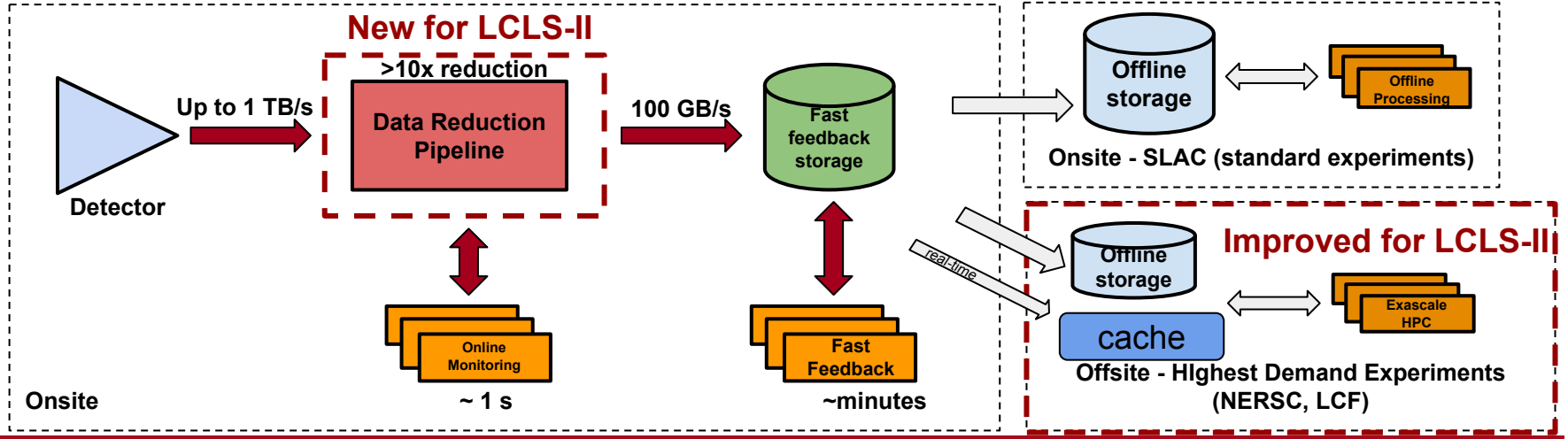


# LCLS-I in Numbers

- about 2000 registered LCLS users
- about 25% of proposed experiments are accepted
- 150-200 Experiments per year
- 2-3 PB and 350-450K files per year
- 20 PB of archived data in 2.5 million files collected since 2009
- 250K Runs in total
- ~50M key/value pairs for all Runs
- 4.5 PB storage for raw data
- 1.2 PB  storage for user writable files (scratch, results)
- 120 compute nodes with 1600 cores
- For LCLS-II most of these numbers will go up by x10 - x100

# LCLS-II Data System

- Similar to LCLS-I but:
  - Data rates will increase from few GB/s to up to 1 TB/s
  - **Data needs to be reduced as we can not write everything to disk**
- Events are not built before being written to disk. The detector contributions to an event are distributed over many files.
- Streaming to remote HPC sites
- Expect single file write rate to increase from 200MB/s to ~1-2GB/s

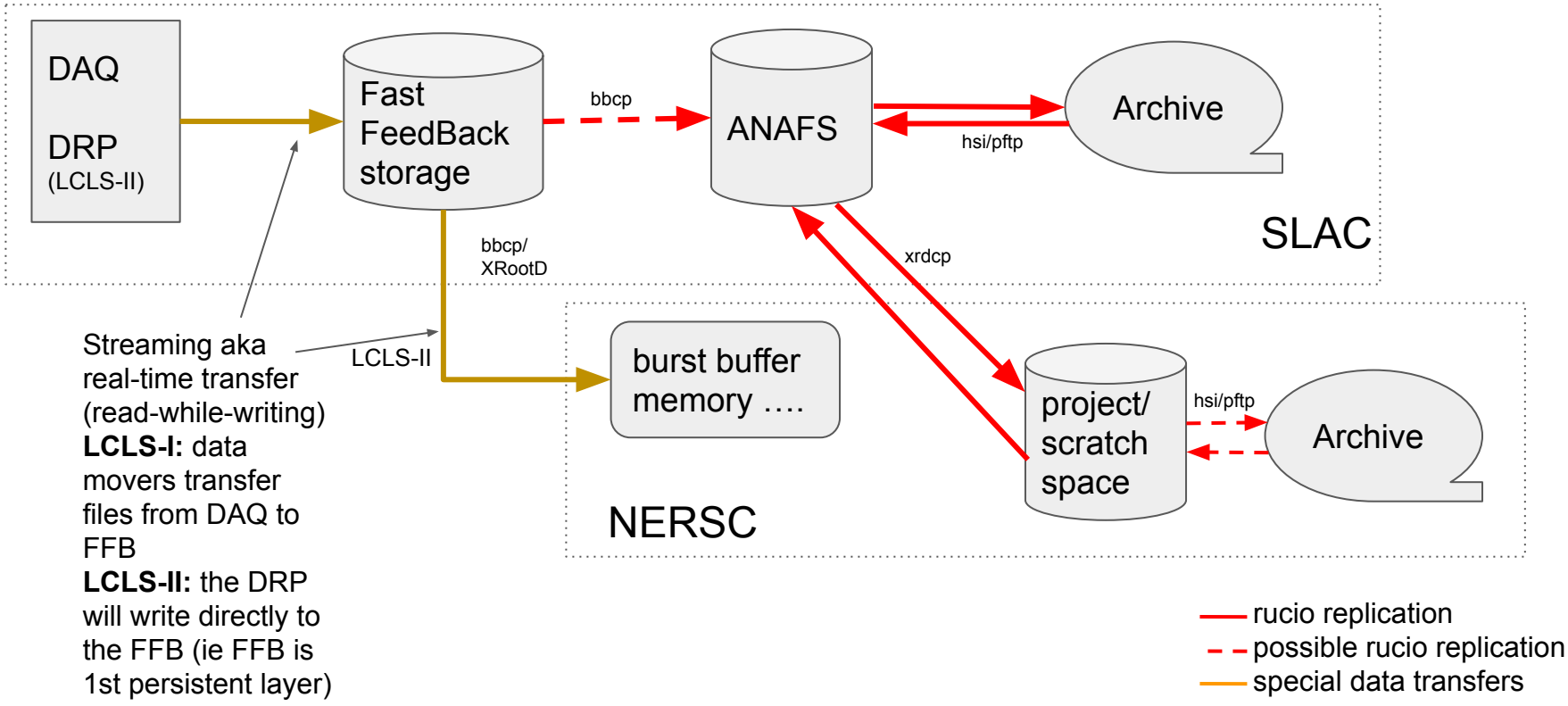



**Data reduction mitigates storage, networking, and processing requirements**

# LCLS Data Management

- The Data Management handles three different data types:
  - raw data in xtc format (grouped into runs, a.k.a **datasets** in Rucio)
    - most files are in this group
  - user daq data (not associated with a run)
    - only collected by a few experiments, files size typically small O(MB)
  - Secondary processed data (could be run associated)
    - example: process and converting raw data to hdf5 format.
- Users access files/runs using a parallel file system (Lustre), files are found by using a predefined path e.g.: /cds/data/psdm/<instr>/<exper>/xtc.
  A user is not directly accessing the file-catalog.
- User created files (during processing/analysis) are not managed by us we just provide disk space

# LCLS - Data Transfers/Replication




**LCLS-I:** data movers transfer files from DAQ to FFB

**LCLS-II:** the DRP will write directly to the FFB (ie FFB is 1st persistent layer)

# Rucio Role in LCLS

- Data Catalog (File Manager)
- File Replication
  - Archive and restore from tape
- Purging files from disk
- Only be used for raw data
- Users don't have direct access to RUCIO
- File count and size
  - total size ~20PB, 2.5 million files
  - ~3PB/year with 300-400K files /year
  - the yearly rates will increase by x20 (2022) - x100 (2028)

| | |
|---|---|
| experiments | ~10K |
| runs (data sets) | millions |
| number of raw data files | 100's of millions over the next 5-10 yr. |

# Configuring Rucio Service Account

- Install git, docker, and docker-compose as pre-requisite tools in development machine
- Clone rucio repos in GitHub: rucio/rucio and rucio/containers
- Prefer SSH over ‘username/password’ authentication method
- As noted in the Policy packages section of Rucio Documentation:
  - rucio/lib/rucio/common/schema/lcls.py (atlas.py as template)
  - rucio/lib/rucio/core/permission/lcls.py (generic.py as template)
    - Set up SSH access for user (ssh-keygen credentials)
      - Add and define perm_get_auth_token_ssh(issuer, kwargs)
      - In has_permission(issuer, action, kwargs), add:
        - 'get_auth_token_ssh': perm_get_auth_token_ssh,
      - In the [client] section of user’s rucio.cfg :
        - auth_type=ssh
        - ssh_private_key=/root/.ssh/id_rsa,
  - rucio/lib/rucio/common/utils.py (implement **non-deterministic** SURL algorithm for LCLS)

# Non-deterministic SURL for LCLS

```
    def construct_surl_LCLS(dsn, filename):
        """
        Defines relative SURL for replicas. This method uses the LCLS convention
        for xtc files. To be used for non-deterministic sites.

        @param: filename of format <instrument>.<experiment><fld>.<remain>
        @return: relative SURL for new replica.
        @rtype: str
        """

        instr, expt, fld, remain = filename.split('.', 3)

        if fld == 'xtc' and filename.endswith('smd.xtc'):
            return '/%s/%s/xtc/smalldata/%s' % (instr, expt, remain)

        return '/%s/%s/%s/%s' % (instr, expt, fld, remain)

register_surl_algorithm(construct_surl_LCLS, 'LCLS')
```

Could have been easier if the scope of the raw data file's DID was made available in /lib/rucio/common/utils.py. (feature request submitted to Rucio team)

# Running RUCIO in Docker Containers

- **# docker build -t rucio/rucio-dev .** (in containers/dev) ⇒ ~900MB rucio/rucio-dev:latest image
- **# docker-compose --file docker-compose.yml up -d** (in rucio/etc/docker/dev)

| IMAGE | COMMAND | PORTS | NAMES |
|---|---|---|---|
| gitlab-registry.cern.ch/fts/fts-monitoring | "/usr/sbin/apachectl…" | 0.0.0.0:8449->8449/tcp | fts_webmon_1 |
| gitlab-registry.cern.ch/fts/fts-rest | "/usr/sbin/apachectl…" | 0.0.0.0:8446->8446/tcp | fts_rest_1 |
| gitlab-registry.cern.ch/fts/fts3:x509-scitokens-issuer-client | "/usr/bin/supervisor…" | 2170/tcp | fts_server_1 |
| mysql:5 | "docker-entrypoint.s…" | 3306/tcp, 33060/tcp | fts_mysql_1 |
| rucio/rucio-dev | "httpd -D FOREGROUND" | 0.0.0.0:80->80/tcp, 0.0.0.0:8443->8443/tcp, 443/tcp | dev_rucio_1 |
| rucio/rucio-ui | "/docker-entrypoint.…" | 0.0.0.0:8444->443/tcp | dev_rucioui_1 |
| postgres:11 | "docker-entrypoint.s…" | 0.0.0.0:5432->5432/tcp | dev_ruciodb_1 |
| graphiteapp/graphite-statsd | "/entrypoint" | 80/tcp, 2003-2004/tcp, 2013-2014/tcp, 2023-2024/tcp, 8125-8126/tcp, 0.0.0.0:8080->8080/tcp, 8125/udp | dev_graphite_1 |

- FTS service configured with xrootd service endpoints for replication
- PostgreSQL (conscious choice for open source DB) configured for the Rucio database backend.

# Validating and Debugging Rucio Installation

- # rucio --version ==> **1.26.1 (Stable)**
- User-oriented Web UI container
- The actual changes for enabling SSH are discovered through debugging the provided unit tests inside the Rucio container:
  - tools/run_tests_docker.sh (take time to run all tests; inundated the DB with test data for validating initial installation! Consider -i option to pick individual unit tests.)
- Run through the examples in the Rucio documentation
- [ToDo] Increase visibility into Rucio Server operation:
  - Run Flask with Rucio app in Debug mode
  - Remote debugger attached to Rucio server in container
    - Visual Studio Code (Free)
    - PyCharm Professional Edition ($)

# Replicating a File from Rucio

1. # rucio list-rse-attributes LCLS_DATA
2. LCLS_DATA: True
3. fts: https://<SLAC IP address>:8446
4. istape: False
5. naming_convention: LCLS
6. # rucio **upload** --rse LCLS_DATA --scope rte01 --name xtc.file.rte01-r0001-s02-c00.xtc --pfn <SLAC pfn> /tmp/rte01-r0001-s02-c00.xtc
7. # rucio **add-rule** psdm:rte.rte01.xtc.rte01-r0001-s02-c00.xtc 1 LCLS_NERSC (similar to LCLS_DATA)
8. Run the rucio daemons --run-once: **judge-evaluator**, **conveyor-[submitter**, **poller**, **finisher]**
9. # rucio **list-file-replicas** --pfns psdm:rte.rte01.xtc.rte01-r0001-s02-c00.xtc
    - root://<SLAC xrootd endpoint>//psdm/rucio//rte/rte01/xtc/rte01-r0002-s02-c00.xtc
    - root://<NERSC xrootd endpoint>//psdm/rucio//rte/rte01/xtc/rte01-r0002-s02-c00.xtc

- Reported BUG: **double slashes** needed in storage **prefix,** highlighted in RED above.
- Question/Issue: why **pfn** necessary (error otherwise) in rucio **upload** when LCLS_DATA already attributed LCLS as non-deterministic naming convention ?

# Testing RUCIO with FTS3 Transfers

- We were able to use FTS 3 with Rucio to drive Third Party Copy (TPC)
  - LCLS will use xrootd TPC with “sss” security module (Simple Shared Secret)
  - We use rucio-conveyor-poller
- FTS3 came in container form from Gitlab @ CERN, including:
  - FTS server (set up is a bit more generic than LCLS need)
    - support xrootd TPC and http TPC: sss and x509 (w/ macaroon for HTTP TPC)
    - The “sss’ key is bind mounted to the container.
  - FTS rest
  - FTS web monitoring
  - MySQL 5 backend
- One issue
  - Rucio uses an X509 proxy to submit to FTS3. This step doesn’t include delegation
  - We need to **manually** delegate a X509 proxy to FTS3, outside of Rucio.
  - Can we merge the two steps to one? Or better, can we submit without using X509?

# More Open Questions

- Better way (rather than using htar out of loop?) in Rucio to transfer large quantity of small files with tracking, especially to tape storage?
- Besides MD5 (option), ADLER32 (default) in Rucio, how about support for CRC32C (for hardware efficiency with Intel SSE 4.2)?
- How best to interface with HPSS tape systems,  e.g. commanding CLI tools?

# Next Steps

1. Test against the 3rd type of docker-compose w/ActiveMQ full monitoring stack.
2. Integration with HPSS tape archives
3. Provision and operate a much larger Rucio installation beyond the pilot stage, with sizable backend DB (and DBA support) mimicking production.

- Onboarding Notes: **https://github.com/slaclab/onboard-rucio.git**