

# Data Management, Workflows, & Scientific Information Systems

Shelly Ren

March 24, 2017

Neutron Day Seminar Series: Data and  
Instrument Software



Dear NScD staff,

The Neutron Sciences Directorate Oracle systems will be unavailable for maintenance during the following dates and times:

· **Tuesday, Jan 24th, from 11 a.m. to 3 p.m.:** **Accelerator PROD database**  
**Systems impacted:** Accelerator Operations Administration/Bypass Request, Diagnostics/Physics applications, Document Number Reservation, Electronic Logbook, eMod, ICS NetReg, ISDD Portal, Inventory Control, MPS Trips, MPS Audits, PSSO Wireless Handheld Meter Readings Entry, PSSO Meter Readings Report, Power Supply configuration generation, PV Logger, RF Cavity trips, SCORE, SNS channels/status, SNS Service Request Web Interface, SNS Work Order Closeout, and Web reports including ROCS.

**Accelerator operations**

· **Monday, Jan 30th, from 9 a.m. to 1 p.m.:** **SCPROD database**  
**Systems impacted:** ICAT, Instrument alarm application, Channel Archiver, Legacy translation monitor, and SNS instrument monitor.

**Science operations**

· **Tuesday, Jan 31st, from 1 p.m. to 5 p.m.:** **XPROD and COTS databases**  
**Systems impacted:** IPTS including User Survey, ITEMS, Express, PuSH, SAC, IHC Operations, IHC Activities, and XWHOS, IPTS information on Guest Port, Sample Environment equipment report, DataStream, ProjectWise, and Primavera.

**User Program; Asset, document management**

If you have any questions or concerns, please contact us at [sisupport@ornl.gov](mailto:sisupport@ornl.gov).

Yours,

Scientific Information Systems Team

# Improved Work Control System

Work  
Planning

Work  
Request

Work  
Order

Chestnut Ridge Service Request System

Submit Work Request

My Requests

My Work Orders

Requests to Screen

Work Overview

Requestor: Shelly Ren

Work Area: Neutron Beam Lines

Requested For: REN, SHELLY

Description: Need vacuum work

Desired Completion Date: 31-Mar-17

Do you know the component/system Asset ID:  Yes  No

Location/Area: 8702 - EXPERIMENTAL HALL - BEAM LINE 2

Cost Object:

Area Manager(s): Bobby Cross Jr, Bradley Horn, Douglas Engle

Additional Email Recipients: Mallamace, Francesco -> 00948989 -> | Mamontov, Eugene -> 00746709 -> 8657711387  
Malliakas, Christos D -> 00965062 -> |  
Malmgren, Thomas W -> 00913046 -> |  
Malone, Steve -> 00909640 -> |  
Mammosser, John -> 00913993 -> |  
Man, Haoran -> 03032943 -> |  
Mancosky, Douglas G -> 00959073 -> |  
Manjon Sanz, Alicia M -> 03034842 -> |  
Mankey, Gary Jay -> 00745960 -> |

Attach File(s): Choose Files No file chosen

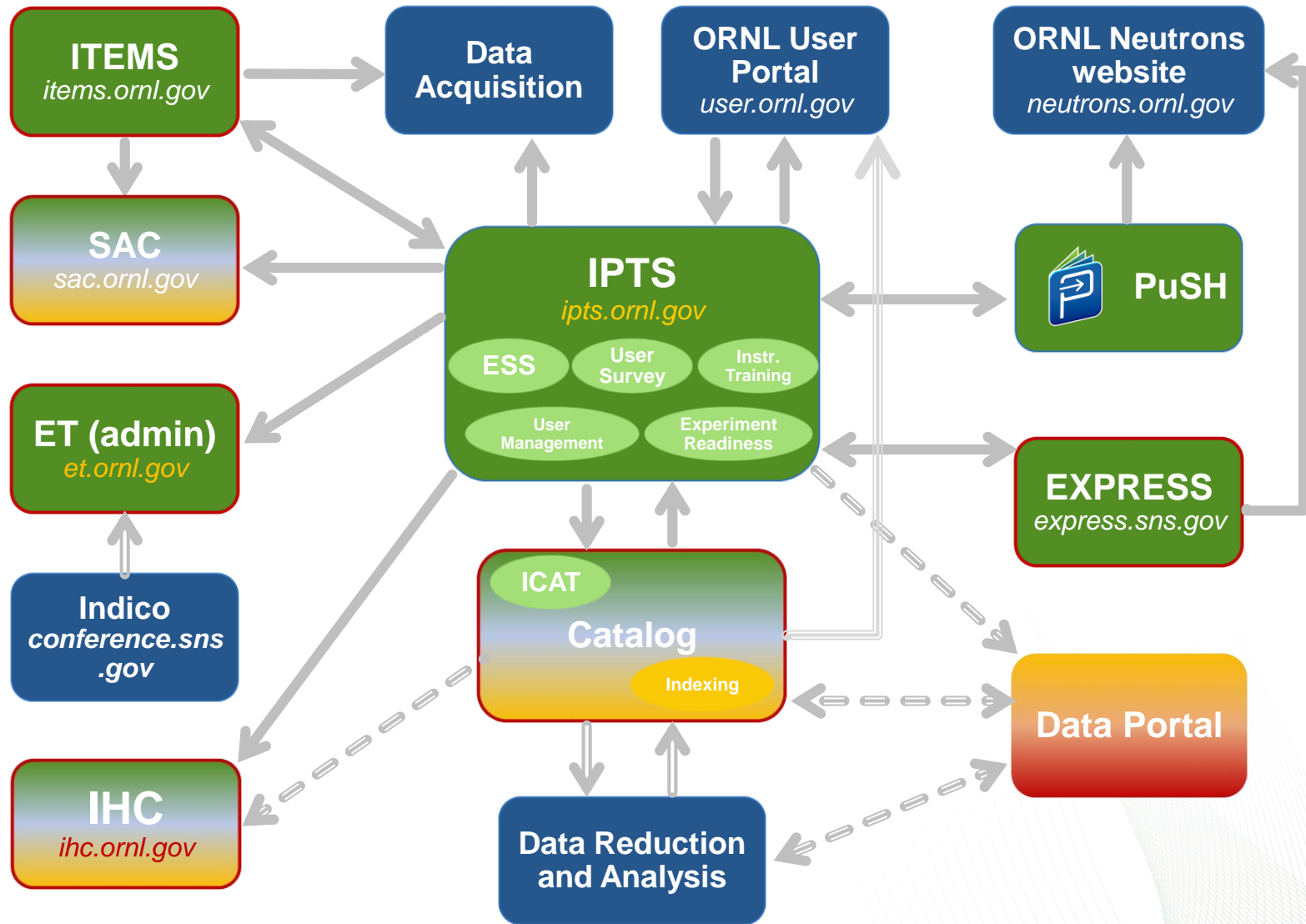
All my work requests data and status

Information on the work order: task leader, group, & status

Work requests are split into five general areas:

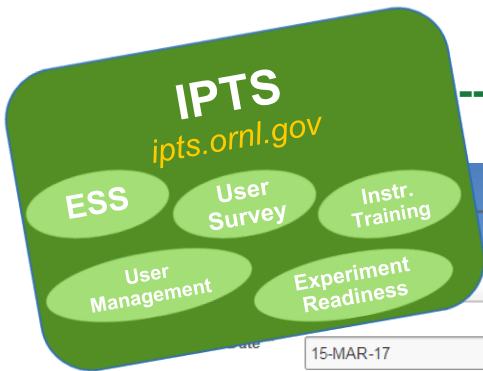
1. "Accelerator" for all work requested for the SNS accelerator
2. "Facility Maintenance" for all building and associated infrastructure work requests in the Chestnut Ridge Complex
3. "Neutron Beam Lines" for all work requested for the Neutron Beam Lines including associated instruments and support systems
4. "Target" for all work requested for the SNS target systems
5. "Test Facilities" for all OM&S work requested

# Integrated Scientific Information Systems



# Integrated Scientific Information Systems

## Integrated Proposal Tracking System (IPTS)



TRACKING SYSTEM

3qr Home All Proposals

Start Date: 15-MAR-17 End Date: 29-MAR-17

Search: [ ] Go Actions

- Experiment planning
- ORCID integration
- DOI landing page

- Beamline = 'BL-14B'
- APPROVED

Beamline	IPTS#	Instrument Status	Final Safety Review Status	ESS Approved	Instrument Team Safety Rev	Sample Management (SMA)	Instrument Specific Training	Review and Sign ESS	Scheduled Start Date	Scheduled End Date	
BL-14B	<a href="#">IPTS-17754.1</a>	<a href="#">Approved</a> <a href="#">Confirmed</a>	SNS - Acceptable	Douglass Rowland					13-MAR-17	21-MAR-17	EXOTIC MONOPOLE DYNAM OXYGEN DEFICIENT Dy2T2O
BL-14B	<a href="#">IPTS-17837.1</a>	<a href="#">Approved</a> <a href="#">Confirmed</a>	SNS - Acceptable	Douglass Rowland					22-MAR-17	28-MAR-17	Investigation of intrinsic localiz of PbSe

1 - 2

**My Instrument Experiment Confirmation Progress**

Search IPTS: [ ] Go

Details	View Confirmation	IPTS-	All Instruments	Proposal Date	Type	Title	Lab
		IPTS-828.1	Bio-SANS, GP-SANS	28-JAN-08	CALIBRATION	Beamline calibration activities	<a href="#">Complete</a>
		IPTS-5908.1	BASIS	15-AUG-11	CALIBRATION	Tests on BL2	<a href="#">Complete</a>



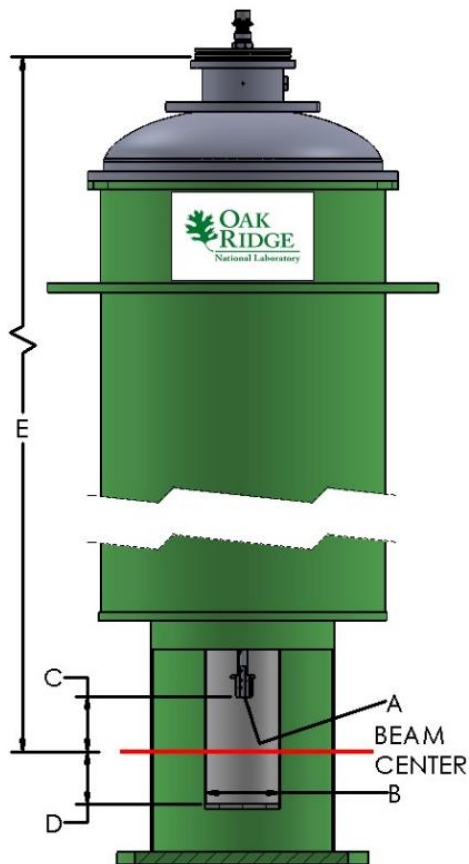
# Integrated Scientific Information Systems

## -- Experiment Resource Scheduling System (EXPRESS)

### CRYO-A

Oxford Instruments Variox

Temp Range: 1.5 to 300K



Description	Value	Units
A Interface Connection	M8	
B Bore Size Diameter	50	mm
C Distance Interface to Beam Center	2.44	in
D Beam Center to Sample Space Bottom	1.92	in
E Distance Stick Flange to Beam Center	46	in

### Sample Environment

- Overview
- Team & Contacts
- Equipment
- Sample Mounting
- Procedures
- User Supplied Equipment
- Useful Links

**This item is available for use at the following:**

Facility:  
HFIR

Associated Instruments:  
CG-1A, CG-2, HB-1, HB-1A, HB-2A, HB-2C, HB-2D, HB-3

**Can be used with the following:**

Associated Resources:  
ULT-B, ULT-G, ULT-K



# Integrated Scientific Information Systems

## -- Publication of SNS and HFIR (PuSH)

[Home](#) | [Login](#) | [Author Home](#) | [All Authors](#) | [NScD Divisions](#) | [ORNL](#) | [Institutions](#) | [Instruments](#) | [Experiments](#) | [Search](#) | [My Reports](#)

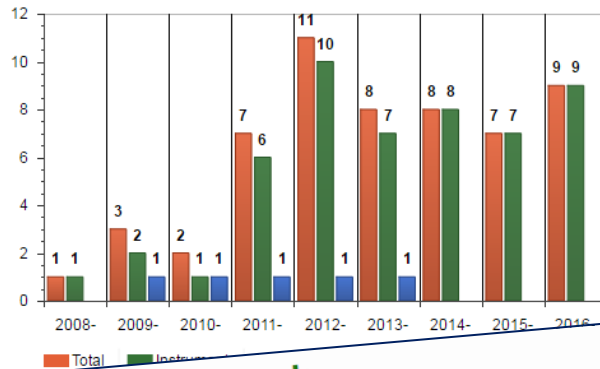
### Valeria V. Lauter

ORNL NScD (Neutron Sciences Directorate)  
Quantum Condensed Matter Division

Total Publications in PuSH: **57**

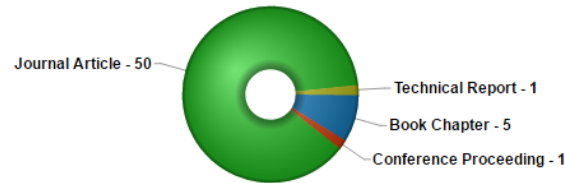
Instrument Publications: **51**

#### PUBLICATIONS BY YEAR



#### PUBLICATIONS BY TYPE

myPuSH for NScD staff



#### INSTRUMENT PUBLICATIONS

Instrument	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	Total
BL-4A	1	2	1	6	10	7	8	7	9		51
BL-4B				1				1	1		3
CG-4C								1			1
BL-1B											
CG-1D											

### Publications Search

Rows 20

	DOI/URL	Publication
View		P. E. Aba-Perea, T. Pirling, M. Preuss, "In-situ residual stress analysis during annealing treatments using neutron diffraction in combination with a novel furnace design." <i>Materials &amp; Design</i> 110, 925-931 (2016).
View		M. N. Abdelmalak, "MXenes: A New Family of Two-Dimensional Materials and its Application as Electrodes for Li-ion Batteries." Ph.D. Dissertation, Drexel University (2014).
View		H. A. Abderrahim, J. Galambos, Y. Gohar, S. Henderson, G. Lawrence, T. McManamy, A. C. Mueller, S. Nagaitsev, J. Nolen, E. Pitcher, R. Rimmer, R. Sheffield, M. Todosow, "Accelerator and target technology for accelerator driven transmutation and energy production." Fermi Laboratory, FERMILAB-FN-0907-DI (September 2010).



# Integrated Scientific Information Systems

## -- Engagement Tracking Tool (ET)

Engagement Tracking Tool

- Home
- Events
- Participants
- Dialogs
- Data Types
- Report Builder
  - Event Breakdown
  - Institution Breakdown
  - Industry Questionnaire
  - Instrument User Summary
- Activity Log

### 2015 17th National School on Neutron and X-Ray Scattering (NXS) Breakdown

Event ID: 2015 17th National School on Neutron and X-Ray Scattering (NXS) (13-JUN-15)

Event ID	NXS2015
Event Name	2015 17th National School on Neutron and X-Ray Scattering (NXS)
Description	
Location	SNS/HFIR
Start Date	13-JUN-15
End Date	27-JUN-15
Event Type ID	NXSchool
Host Institution	ORNL NScD (Neutron Sciences Directorate)
Attendance	61 Participants

### On Site Users Related to 2015 17th National School on Neutron and X-Ray Scattering (NXS)

	Unique Users	Total Visits
Total Associated Users (both HFIR and SNS)	50	219
Users at ORNL prior before and after	16	111
Users at ORNL only prior to NXS2015	34	108
Users at ORNL only after NXS2015	0	0

	Unique Users	Total Visits
Users at HFIR both before and after NXS2015	16	53
Users at SNS both before and after NXS2015	16	58

51

**Number of Institutions Sending Participants**

---

0

**Number of Events subsequently attended by these Participants**

---

0

**Total Number Participants Going to Subsequent Events**

---

113

**Total Number of Proposals submitted after Event**

---

41

**Completed Proposals submitted after Event**

---

23

**Proposals Accepted but Not Awarded Time submitted after Event**

---

49

**Other Proposal Types (Not Accepted) submitted after Event**

---

9

**Number of Publications Published after Event**





# Integrated Scientific Information Systems

## -- Instrument Hall Coordinator System (IHC)

### Operations

- View Archive
- IHC Reports
- Administrative Actio...
- User Notifications
- Registered SNS Addresses
- Registered HFIR Addresses
- Manage Application Roles
- Update Downtime
- Add New Activities
- List Activities
- Beam on Sample
- HFIRLog
- Home

Log Activity for Date \*  
 22-MAR-2017  
 (today)

Shift \*  
 Day  Night

Production Beam to Target  
 4.1 Neutron Production Beam Hours

Shift Summary/Comments \*  
 Brian Plante is the on shift instrument hall coordinator (865)241-4432. The beam target at 60 Hz, 1.01 MW, HFIR is down for scheduled maintenance.

152 of 4000

IHC on Shift Brian Plante

- Log IHC specific activities
- Log notable events/issues and update SNS/HFIR eLogs
- Send notifications to users on any significant beam status changes
- Record instrument downtime

Lower sample area, if level is less than 45%, IHC will switch system over to a dewar.

Added new cave rad monitor (far west) to alarm handler for BL-11a. The far west has a 1mR and 2mR alarm set point. There is guidance for both alarm in the "what to do section".

Wednesday night-BL16b staff request we turn ON the tan sample environment compressor 06:00.

What's New

New CSS alarms for MaNDi have been entered into the IHC alarm handler, the timing PV is disconnected and has been disabled.

Added new cave rad monitor (far west) to alarm handler for BL-11a. The far west has a 1mR and 2mR alarm set point. There is guidance for both alarm in the "what to do section".

The BL-16B (Detector:HE Comp) alarm has been disabled for the outage.

Newest version of CSS has been loaded at the IHC workstation. Some older CSS screens may display improperly for the interim, if you observe a screen with an improper display notify ky9@ornl.gov. In addition you will notice a few changes--to

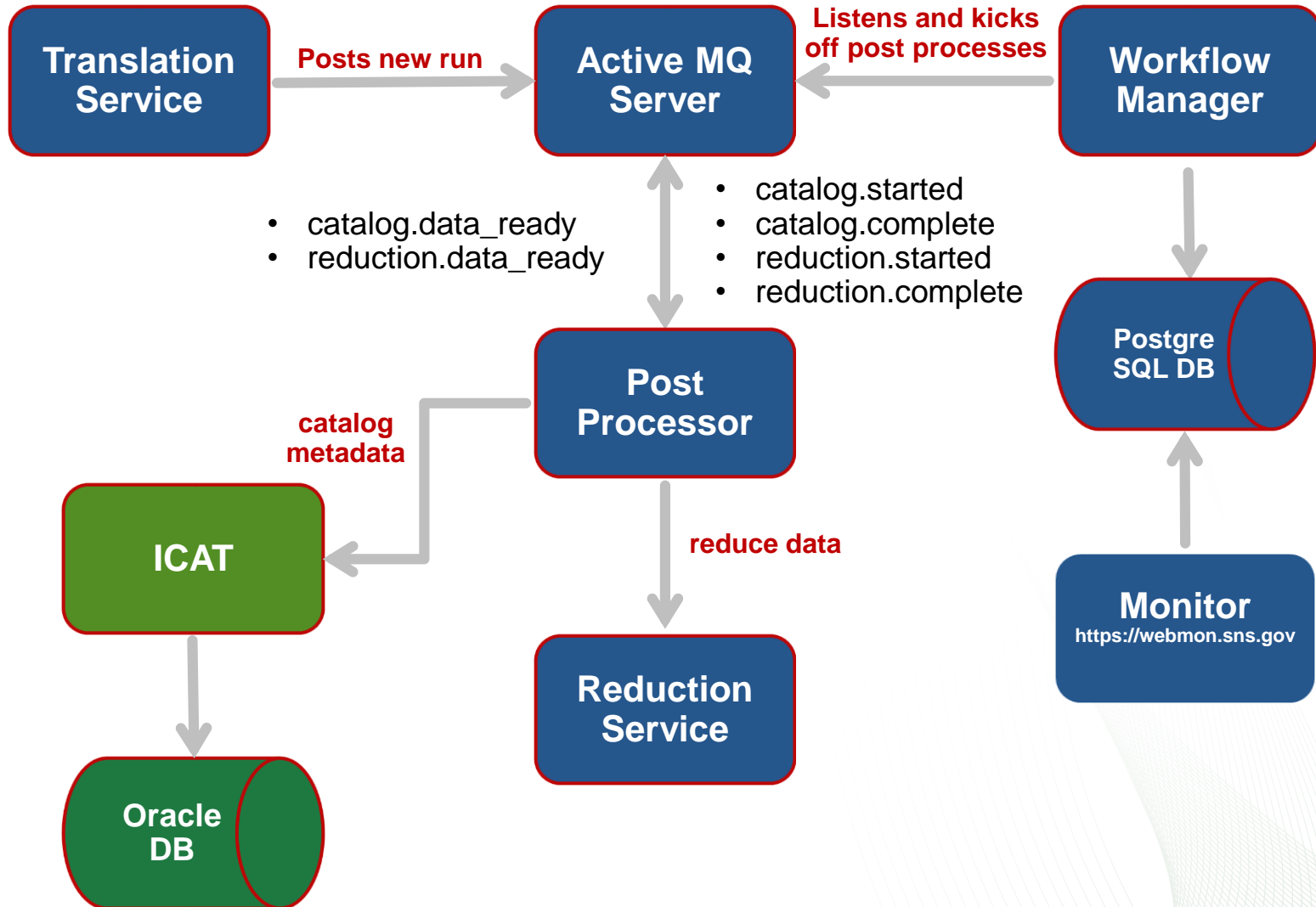
Log Book Status

Category \*  
 Beamline 01A - USANS

Group  
 ADARA  
 CLO (8600)  
**Chopper**  
 Data Access  
 Data Acquisition System

Comments  
 The T-0 chopper was running and phase locked.

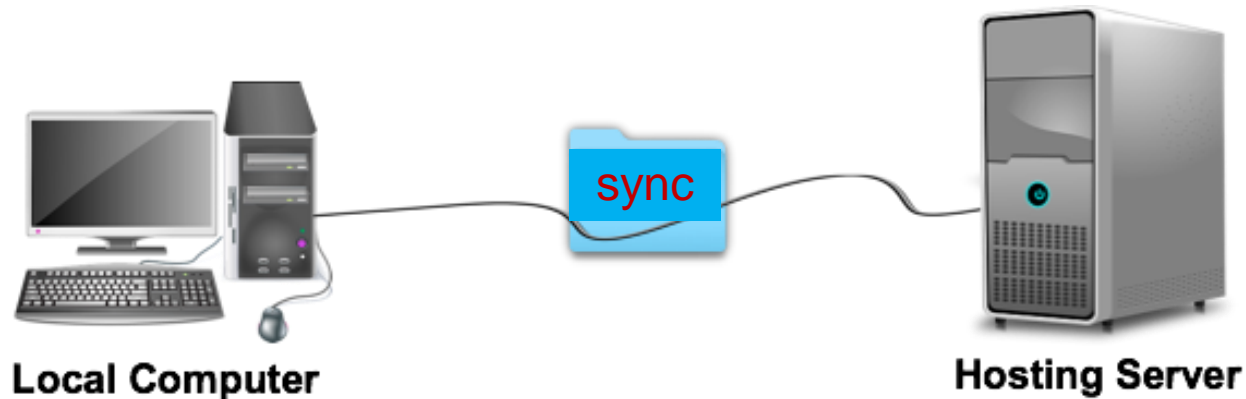
# Data Management and Workflows @ SNS



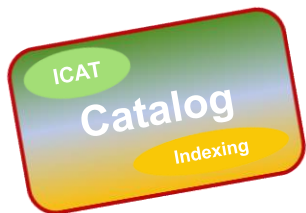
# Data Management and Workflows

## -- Data archiving tool

- Create IPTS and shared directories for scheduled experiments
- Reset permissions for given instrument & IPTS



- Archive data for HFIR instruments by syncing files from "source" to "destination" directories
- Apply ACL / permissions set
- **Catalog metadata per instrument's "catalog policy"**



# Data Management and Workflows

## -- Catalog System

Web services designed for NDAV applications

- New services:
- Provide metadata for portal users
  - Index metadata to enable free text search

### ORNL Data Catalog API

API to store and query ORNL datafile metadata.

#### facilities

Show/Hide | List Operations | Expand Operations

GET	/facilities/
GET	/facilities/{facility}/
GET	/facilities/{facility}/instruments/

Parameters

Parameter	Value	Description	Parameter Type	Data Type
facility	<input type="text" value="(required)"/>	The name of the facility.	path	string

Response Messages

HTTP Status Code	Reason	Response Model	Headers
200	Success		

GET	/facilities/{facility}/instruments/{instrument}/
GET	/facilities/{facility}/instruments/{instrument}/experiments/
GET	/facilities/{facility}/instruments/{instrument}/experiments/{experiment}/
GET	/facilities/{facility}/instruments/{instrument}/experiments/{experiment}/datafiles/
GET	/facilities/{facility}/instruments/{instrument}/experiments/{experiment}/datafiles/{datafile}/
PUT	/facilities/{facility}/instruments/{instrument}/experiments/{experiment}/datafiles/{datafile}/
GET	/facilities/{facility}/instruments/{instrument}/experiments/{experiment}/exts/
GET	/facilities/{facility}/instruments/{instrument}/experiments/{experiment}/tags/

# Data Management, Workflows, & Scientific Information Systems

## -- Initiatives, ideas and path forward

- Usability study and expert evaluation of web applications
- Data Science - Analysis/Analytics/Intelligence
  - Equipment usage (i.e. sample environment)
  - Publications / beam line
  - Institutions representation and productivity
- A new data portal
  - Globus API for data transfer
  - Remote jobs
  - Metadata annotation
  - DOI on demand for PIs to publish datasets



Please feel free to contact us at [sisupport@ornl.gov](mailto:sisupport@ornl.gov).