



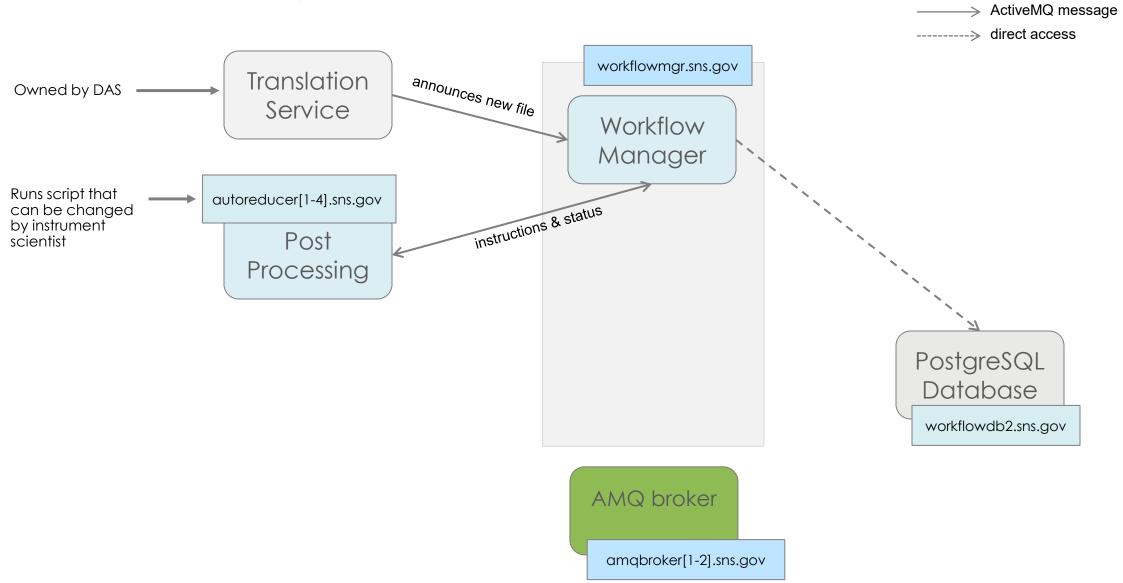
ORNL is managed by UT-Battelle LLC for the US Department of Energy



Event data "translation" to Nexus file Cataloging Cataloging Auto reduction https://monitor.sns.gov/

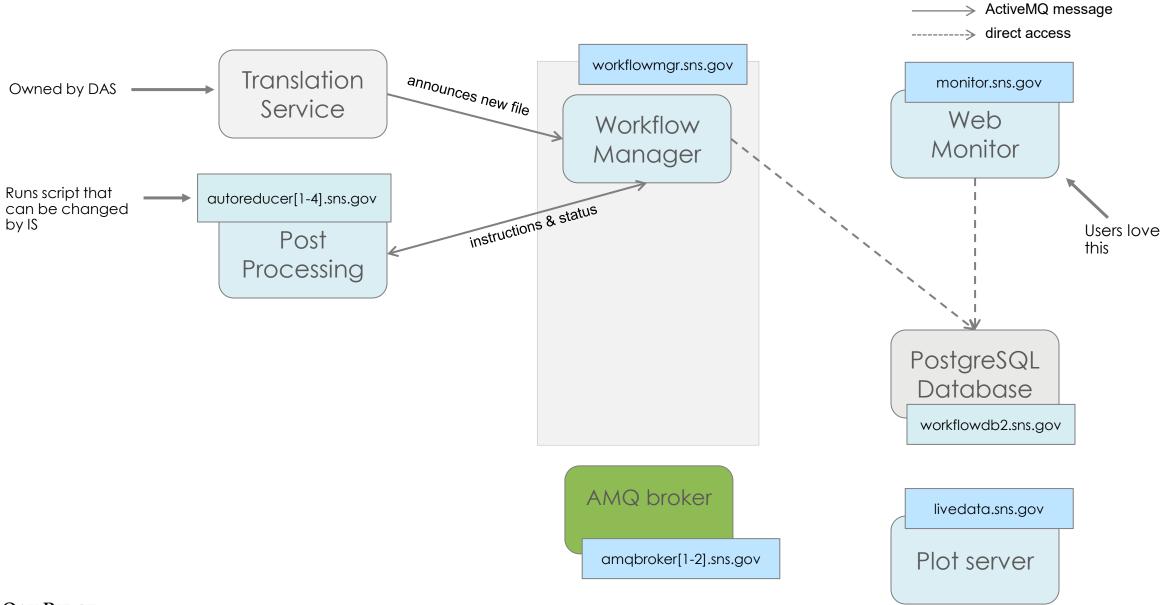
- Originally, "translation" to Nexus files was done after a run completed and took a lot of time
- Around 2012, the ADARA project changed everything to event streaming
 - "Translation" now starts at the beginning of the run
- As part of that effort, the automated reduction workflow was created
 - The web monitor was initially a diagnostics tool for developers but quickly became popular

Post-Processing Architecture

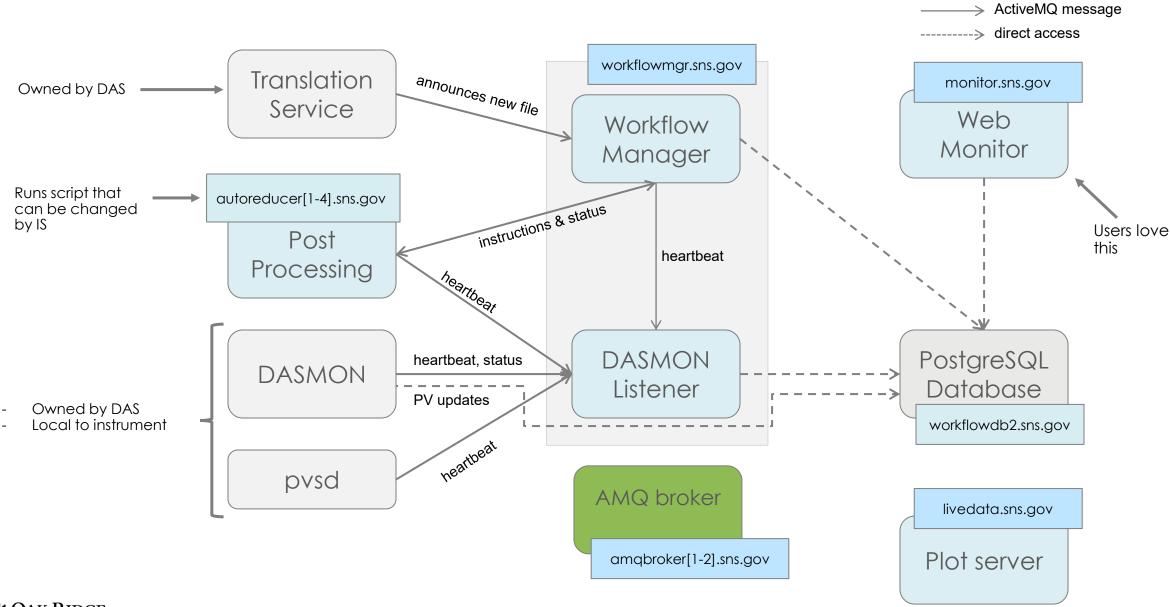




Post-Processing Architecture

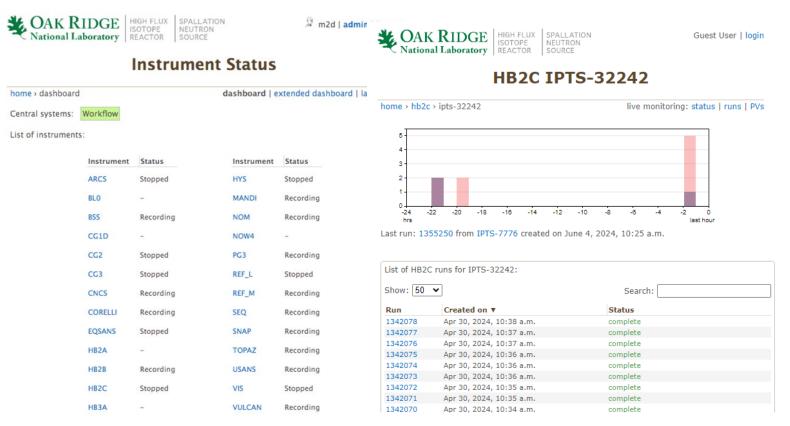


Post-Processing Architecture



Web monitor – monitor.sns.gov

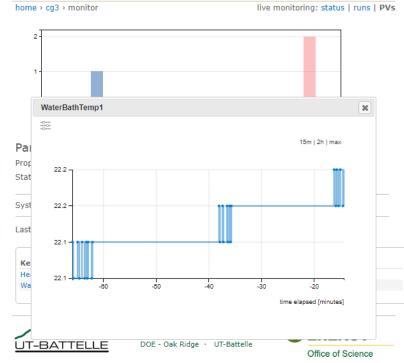
User-facing part of WebMon





Guest User | login

CG3 Process Variables

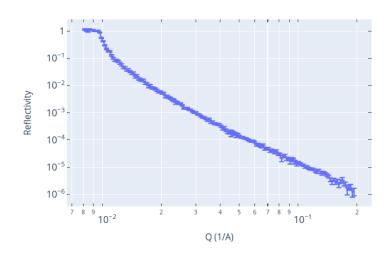


Web monitor – monitor.sns.gov

Rerun cataloging and reduction

REF L Run 208109





Configure autoreduction (IS only)

CNCS Configuration

		Configuring th	ne automate	ed reduction —		
Instrument team	members ca	an use this page	to generate	a new automate	d reduction s	cript.
 Click the 	reset to pop	ulate the form w	ith default va	d reduction script dues. ritten once you c		it button.
st of parameters for	CNCS reduc	ction template:				
Raw vanadium	/SNS/CNCS//PTS-28950/nexus/CNCS_449014.nxs.h5					
Processed vanadium	van_449014.nxs					
Output directory						
Vanadium integration	min	49501.0	max	50501.0		
Motor names	omega					
Temperature names	$\fbox{Sample Temp, sample temp, Sensor B, Sensor A, temp 5, temp 8, sensor 0r}$					
Grouping file	powder 🗸					
Create elastic nxspe						
Create MD nxs						
Energy in meV						
Energy binning	E _{min}	-1.0	E _{step}	0.005	E _{max}	0.95
TOF offset	t ₀ [Auto-fit t ₀ to	get E=0 at elas	tic peak 🗌	
Time independent bck	min		max		Perform TIE	3 🔽
UB matrix	a[4.54	b	4.54	С	11.862
	alpha	90.0	beta	90.0	gamma	120.0
	u_vector[-0.1019, -0.01	v_vector	1.0000, 0.018		
Masked Bank	M	lasked Tube		Masked Pixel		0
				124-128		ŵ
				1-4		ŵ
						ŵ
36-50						_
36-50						submit re



Technologies

- ActiveMQ Classic message broker
- Python clients using the STOMP messaging protocol
 - Workflow manager
 - Dasmon listener
 - Autoreducer
- 2 Django apps
 - Web monitor (monitor.sns.gov)
 - Live Data Server (livedata.sns.gov)
- 2 PostgreSQL databases (workflowdb2.sns.gov and livedata.sns.gov)



Autoreducers / post-processing agent

- Repo: https://github.com/neutrons/post_processing_agent
- Postprocessing tasks it handles:
 - Cataloging of raw data in ONCat (https://oncat.ornl.gov/)
 - Users can download their data from ONCat
 - Autoreduction
 - Runs instrument-specific data reduction script
 - Publishes plots to Live Data Server
 - Cataloging of reduced data in ONCat
 - Adjusting parameters in the autoreduction scripts (available to instrument scientists)
- 4 instances running on autoreducer[1-4].sns.gov



Testing strategy

- Unit tests
- System tests part of CI and for local development
 - System of 11 docker containers for message broker, clients, DB, web server etc.
 - https://github.com/neutrons/data_workflow/blob/next/docker-compose.yml
- Developer test environment in CADES webmon-test.ornl.gov
 - https://code.ornl.gov/sns-hfir-scse/infrastructure/neutrons-test-environment
- https://data-workflow.readthedocs.io/en/latest/developer/index.html



RHEL 7 – RHEL 9 upgrade

- The SNS/HFIR servers were running Red Hat Enterprise Linux 7 (RHEL 7) (EOL: 2024-06-30)
- Neutrons Data Project responsibility: port our (mainly data reduction) software from RHEL 7 to RHEL 9
- Python 2 is not distributed with RHEL 9
- Why not containerize everything?
 - Growing tech debt
 - Cyber security!



Porting Post-Processing Agent

- Removed obsolete code
- Added integration tests with containerized ActiveMQ broker and agent
- Migrated from Python 2.7 to Python 3.9 (RHEL 9 default Python version)
- Still distributed as RPM (RPM Package Manager)



Porting Live Data Server

- Serves plots to monitor.sns.gov
- Production instance used Apache HTTP Server, but initial work had been done in the test environment to move to Nginx and containerize Live Data Server
- Migrated from Python 2.7 + Django 1.9 to Python 3.6 + Django 2.0
 - Story in the backlog to move to latest Python, Django and PostgreSQL
- Tested new RHEL 9 production with WebMon test environment
- Purged old data to shrink PostgreSQL DB from 1.4 TB to 550 GB



Migration from ActiveMQ Classic to ActiveMQ Artemis

- Main difference was message addressing and routing
- Classic has queues (point-to-point) and topics (publishsubscribe)
- Artemis only has queues and uses addresses to achieve different routing mechanisms.
 - Multicast routing: all subscribers to the address get their own queue
 - Anycast routing: only one queue for the address that all consumers subscribe to
- https://activemq.apache.org/components/artemis/migration-documentation/



Thank you!

