

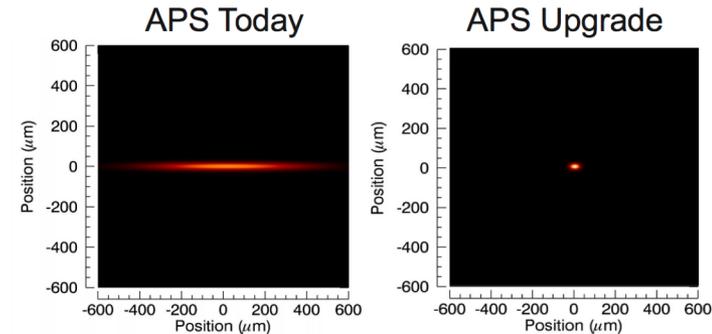
Advanced Photon Source Data Management

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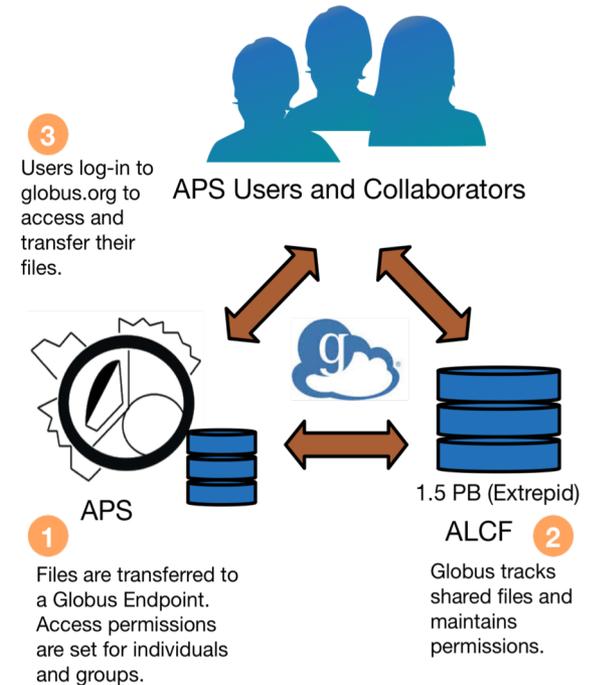
Growing Beamline Data Needs

- X-ray detector capabilities are constantly improving: bigger frames, higher frame rates => more raw data
- APS Upgrade: Higher brightness => more x-rays can be focused onto a smaller area => more raw data in greater detail and less time
- APS 1ID:
 - Today: 4x Hydra GE detector, 8MB frame, 8 fps => 256MB/s data rate (1TB/hr)
 - Production Data Rates (including overhead, on a good week): 10TB/day, 60TB/week
 - Near future (1-3 years): 2x 2923 Dexela (or similar), 23MB frame, 26 fps => 1.2GB/s data rate
 - Near future: Pilatus 2M (or similar/larger), 9.5MB frame, 250 fps => 2.3GB/s data rate
- APS 8IDI:
 - 2010-2016: ANL/LBL FCCD, 2MB frame, 100fps, compressed in real-time with 10% non-zero pixels on the average => about 200MB/s data rate
 - 2016-Today: Lambda 750K, 1.5MB frame, about 10% non-zero pixels, 2000 fps => about 300 MB/s data rate
 - Production Data Rates: 8-10 TB/week (max), 1-2TB/week (average)
 - Future: research on VIPIC (>1MHz frame rate) and UFXC (50 kHz frame rate)

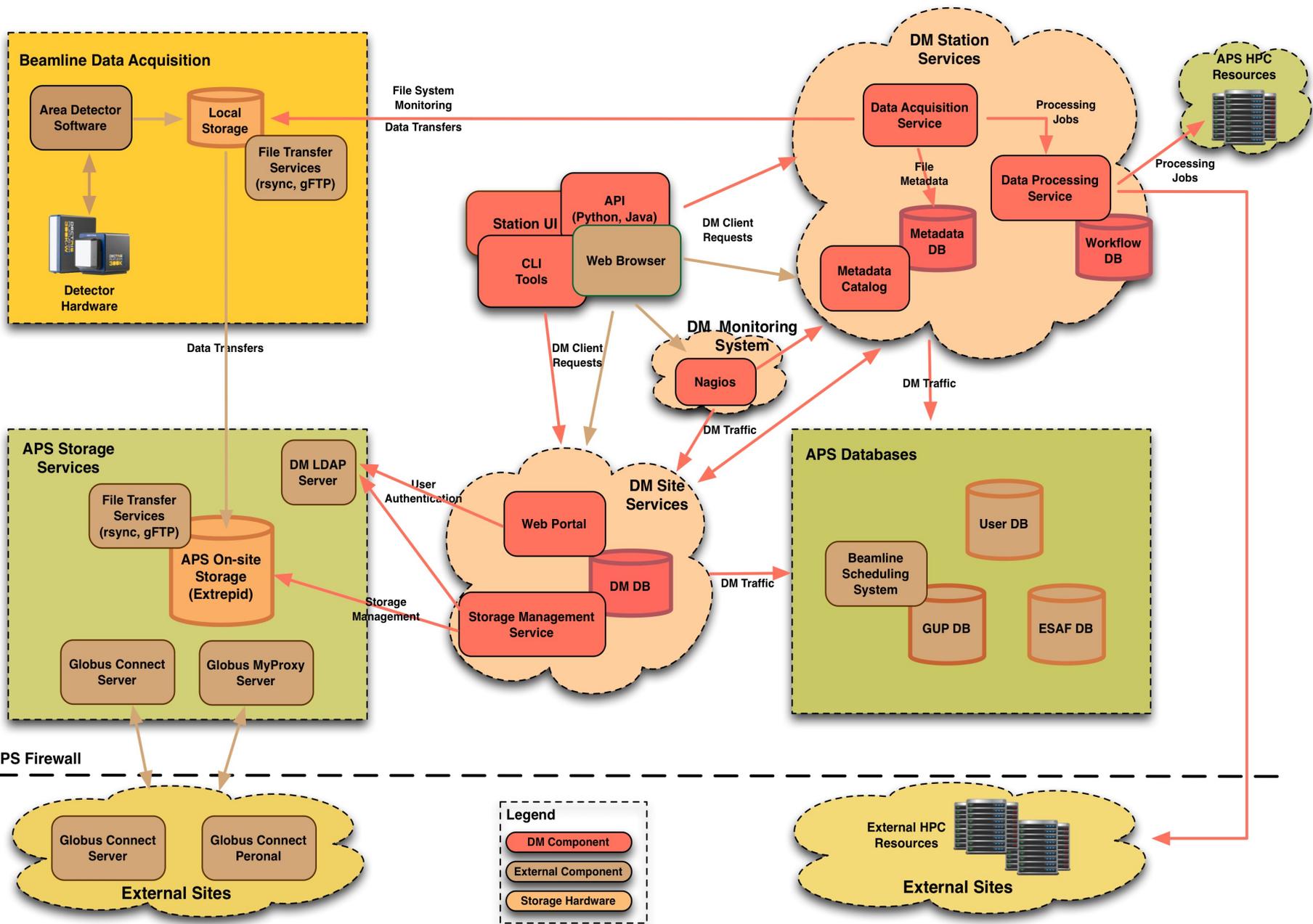


APS Data Management

- Specific data management needs typically vary from beamline-to-beamline, mostly depending upon the types of detectors, X-ray techniques, and data processing tools in use
- However, most of the data management requirements are related to a set of tasks common to all beamlines:
 - Storage area management (e.g. movement of acquired data from local storage to a more permanent location, data archival, etc.)
 - Enabling users and applications to easily find and access data (metadata and replica catalogs, remote data access tools)
 - Facilitating data processing and analysis with automated or user-initiated processing workflows
- APS Data Management (DM) project strives to help with these tasks

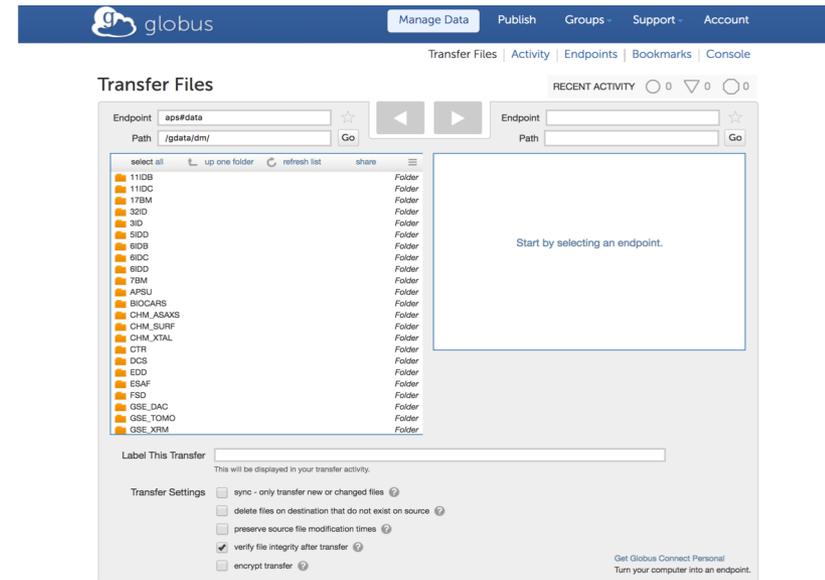


APS Data Management System



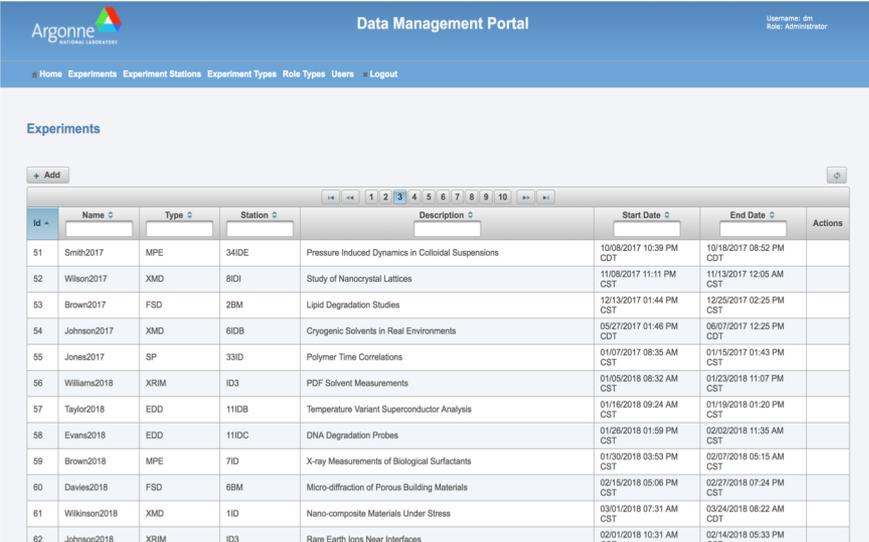
How Does Globus Fit In?

- Globus Connect Server: provides remote data access to APS on-site storage (via the `aps#data` endpoint)
- Globus MyProxy OAuth Server: handles `aps#data` endpoint authentication
- GridFTP servers and clients: used by DM software for internal data transfers between beamline (local) storage and APS on-site storage, for transfers between local storage and HPC resources, etc.
 - Issue: Support for Open Source Globus Toolkit ended in early 2018



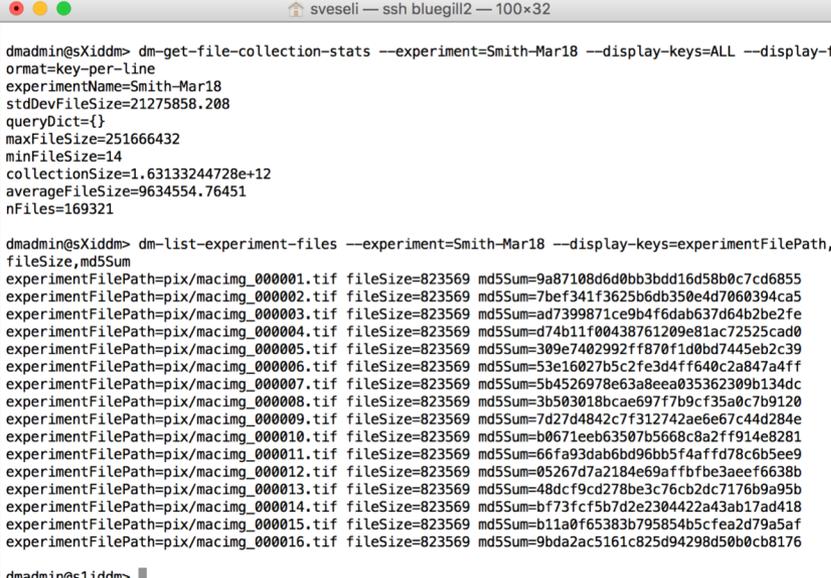
Services

- Site Services:
 - DM Database (PostgreSQL)
 - Storage Management Service
 - Web Portal
 - Automated user account synchronization utilities
- Station (Beamline Deployment) Services:
 - Data Acquisition Service
 - Metadata Catalog
 - Processing Service
- All services are available via REST interfaces



The screenshot shows the Argonne Data Management Portal interface. At the top, there is a navigation bar with the Argonne logo and the text "Data Management Portal". Below the navigation bar, there is a breadcrumb trail: "Home Experiments Experiment Stations Experiment Types Role Types Users Logout". The main content area is titled "Experiments" and contains a table with the following columns: "Id", "Name", "Type", "Station", "Description", "Start Date", "End Date", and "Actions". The table lists 12 experiments, each with a unique ID, name, type, station, description, start date, and end date.

Id	Name	Type	Station	Description	Start Date	End Date	Actions
51	Smith2017	MPE	34IDE	Pressure Induced Dynamics in Colloidal Suspensions	10/08/2017 10:38 PM CDT	10/18/2017 08:52 PM CDT	
52	Wilson2017	XMD	8IDI	Study of Nanocrystal Lattices	11/08/2017 11:11 PM CST	11/13/2017 12:05 AM CST	
53	Brown2017	FSD	28M	Lipid Degradation Studies	12/13/2017 01:44 PM CST	12/25/2017 02:25 PM CST	
54	Johnson2017	XMD	6I0B	Cryogenic Solvents in Real Environments	06/27/2017 01:46 PM CDT	06/07/2017 12:25 PM CDT	
55	Jones2017	SP	33ID	Polymer Time Correlations	01/07/2017 08:35 AM CST	01/15/2017 01:43 PM CST	
56	Williams2018	XRIM	ID3	PDF Solvent Measurements	01/05/2018 08:32 AM CST	01/23/2018 11:07 PM CST	
57	Taylor2018	EDD	11IDB	Temperature Variant Superconductor Analysis	01/16/2018 09:24 AM CST	01/19/2018 01:20 PM CST	
58	Evans2018	EDD	11IDC	DNA Degradation Probes	01/26/2018 01:59 PM CST	02/02/2018 11:35 AM CST	
59	Brown2018	MPE	7ID	X-ray Measurements of Biological Surfactants	01/30/2018 03:53 PM CST	02/07/2018 05:15 AM CST	
60	Davies2018	FSD	68M	Micro-diffraction of Porous Building Materials	02/15/2018 05:06 PM CST	02/27/2018 07:24 PM CST	
61	Wilkinson2018	XMD	1ID	Nano-composite Materials Under Stress	03/01/2018 07:31 AM CST	03/24/2018 08:22 AM CST	
62	Johnson2018	XRIM	ID3	Rare Earth Ions Near Interfaces	02/01/2018 10:31 AM CST	02/14/2018 05:33 PM CST	



The screenshot shows a terminal window with the following output:

```
dmadmin@sXiddm> dm-get-file-collection-stats --experiment=Smith-Mar18 --display-keys=ALL --display-format=key-per-line
experimentName=Smith-Mar18
stdDevFileSize=21275858.208
queryDict={}
maxFileSize=251666432
minFileSize=14
collectionSize=1.63133244728e+12
averageFileSize=9634554.76451
nFiles=169321

dmadmin@sXiddm> dm-list-experiment-files --experiment=Smith-Mar18 --display-keys=experimentFilePath,
fileSize,md5Sum
experimentFilePath=pix/macimg_000001.tif fileSize=823569 md5Sum=9a87108d6d0bb3bdd16d58b8c7cd6855
experimentFilePath=pix/macimg_000002.tif fileSize=823569 md5Sum=7bef341f3625b6db350e4d7060394ca5
experimentFilePath=pix/macimg_000003.tif fileSize=823569 md5Sum=ad7399871ce9b4f6da6b37d64b2be2fe
experimentFilePath=pix/macimg_000004.tif fileSize=823569 md5Sum=d74b11f00438761209e81ac72525cad0
experimentFilePath=pix/macimg_000005.tif fileSize=823569 md5Sum=309e7402992ff870f1d0bd7445eb2c39
experimentFilePath=pix/macimg_000006.tif fileSize=823569 md5Sum=53e16027b5c2fe3d4ff640c2a847a4ff
experimentFilePath=pix/macimg_000007.tif fileSize=823569 md5Sum=5b4526978e63a8eea035362309b134dc
experimentFilePath=pix/macimg_000008.tif fileSize=823569 md5Sum=3b503018bcae697f7b9cf35a0c7b9120
experimentFilePath=pix/macimg_000009.tif fileSize=823569 md5Sum=7d27d4842c7f312742ae6e67c44d284e
experimentFilePath=pix/macimg_000010.tif fileSize=823569 md5Sum=b0671eeb63507b5668c8a2ff914e8281
experimentFilePath=pix/macimg_000011.tif fileSize=823569 md5Sum=66fa93dab6bd96bb5f4affd78c6b5ee9
experimentFilePath=pix/macimg_000012.tif fileSize=823569 md5Sum=05267d7a2184e69aff7bfe3aee6f6638b
experimentFilePath=pix/macimg_000013.tif fileSize=823569 md5Sum=48dcf9cd278be3c76cb2dc7176b9a95b
experimentFilePath=pix/macimg_000014.tif fileSize=823569 md5Sum=bff73cf5b7d2e2304422a43ab17ad418
experimentFilePath=pix/macimg_000015.tif fileSize=823569 md5Sum=b11a0ff65383b795854b5cfea2d79a5af
experimentFilePath=pix/macimg_000016.tif fileSize=823569 md5Sum=9bda2ac5161c825d94298d50b0cb8176

dmadmin@s1iddm> |
```

Monitoring

- Every DM service has a set of monitoring interfaces that enable external applications to find out about its state
- These are used by the custom Nagios plugins that provide up-to-date information about the health of the DM station deployments

Nagios
 Last Updated: Mon Dec 18 08:57:23 CST 2017
 Updated every 90 seconds
 Nagios® Core™ 4.3.4 - www.nagios.org
 Logged in as dmadmin

Current Network Status
 View Service Status Detail For All Service Groups
 View Status Summary For All Service Groups
 View Service Status Grid For All Service Groups

Host Status Totals

Up	Down	Unreachable	Pending
21	0	0	0

All Problems All Types
 0 21

Service Status Totals

Ok	Warning	Unknown	Critical	Pending
69	0	0	0	0

All Problems All Types
 0 69

Service Overview For All Service Groups

DM 11IDB Services (dm-11idb-services)

Host	Status	Services	Actions
s11idbm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 11IDC Services (dm-11idc-services)

Host	Status	Services	Actions
s11idcdm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 17BM Services (dm-17bm-services)

Host	Status	Services	Actions
s17bmdm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 1ID Services (dm-1id-services)

Host	Status	Services	Actions
s1iddm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 32ID Services (dm-32id-services)

Host	Status	Services	Actions
s32iddm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 33ID Services (dm-33id-services)

Host	Status	Services	Actions
sis.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 34IDE Services (dm-34ide-services)

Host	Status	Services	Actions
hpcs34.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 35ID Services (dm-35id-services)

Host	Status	Services	Actions
dcspc53.dcs.aps.anl.gov	UP	3 OK	[Icons]

DM 3ID Services (dm-3id-services)

Host	Status	Services	Actions
s3iddm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 5IDD Services (dm-5idd-services)

Host	Status	Services	Actions
watercress1.dnd.aps.anl.gov	UP	3 OK	[Icons]

DM 6BM Services (dm-6bm-services)

Host	Status	Services	Actions
s6bmdm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 6IDB Services (dm-6idb-services)

Host	Status	Services	Actions
s6idbdc.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 6IDC Services (dm-6idc-services)

Host	Status	Services	Actions
s6iddm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 7BM Services (dm-7bm-services)

Host	Status	Services	Actions
s7bmdm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 7ID Services (dm-7id-services)

Host	Status	Services	Actions
s7iddm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 8ID Services (dm-8id-services)

Host	Status	Services	Actions
s8idapps-vm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM 8ID1 Services (dm-8id1-services)

Host	Status	Services	Actions
s8id1apps-vm.xray.aps.anl.gov	UP	3 OK	[Icons]

DM Storage Services @ apsddata (dm-apsdata-storage-services)

Host	Status	Services	Actions
apsdata.aps.anl.gov	UP	1 OK	[Icons]

DM Storage Services @ bluegill2 (dm-bluegill2-storage-services)

Host	Status	Services	Actions
bluegill2.aps.anl.gov	UP	1 OK	[Icons]

DM TEST Services @ bluegill2 (dm-bluegill2-test-services)

Host	Status	Services	Actions
bluegill2.aps.anl.gov	UP	3 OK	[Icons]

DM CHMCARS Services (dm-chmcars-services)

Host	Status	Services	Actions
bmw.cars.aps.anl.gov	UP	3 OK	[Icons]

DM Storage Services @ cleo (dm-cleo-storage-services)

Host	Status	Services	Actions
cleo.aps.anl.gov	UP	1 OK	[Icons]

DM TEST Services @ cleo (dm-cleo-test-services)

Host	Status	Services	Actions
cleo.aps.anl.gov	UP	3 OK	[Icons]

DM GSECARS Services (dm-gsecars-services)

Host	Status	Services	Actions
bmw.cars.aps.anl.gov	UP	3 OK	[Icons]

User Interfaces

- Web browser access to DM Web Portal, Nagios web pages, beamline Metadata Catalog, and Globus Online (for remote data access)
- Python REST services are accessible via DM Python and Java APIs
- Processing Service provides OMQ interfaces
- Extensive set of command line tools
 - Built on top of Python APIs
 - Session based
 - Fully scriptable
 - Online usage documentation (accessible via the `-h|--help` options)
- DM Station GUI (C. Schmitz)
 - Implemented in PyQt
 - Uses Python REST APIs
 - Easiest way to start using the system

Wilkinson2018 Settings

Name: Wilkinson2018
 Start Date: 3/1/18 End Date: 3/24/18
 Type: XMD
 Description: Nano-composite Materials Under Stress

Badge	First	Last	Email
1 678912345	Laura	Wilkinson	wilkinson@u...
2 891234567	John	Gray	jgray@anl.gov
3 789123456	Amanda	Greene	agreene@anl...
4 912345678	Kathy	Parkins	kparkins@un...
5 123456789	Patrick	Elmer	pelmer@iit.edu

```

Usage:
  dm-6bm-daq --experiment=EXPERIMENTNAME --data-directory=DATADIRECTORY
  [--duration=DURATION]
  [--dest-directory=DESTDIRECTORY]
  [--upload-data-directory-on-exit=UPLoADDATADIRECTORYONEXIT]
  [--upload-dest-directory-on-exit=UPLoADDESTDIRECTORYONEXIT]
  [--process-hidden]
  [--process-existing]
  [--workflow-name=WORKFLOWNAME --workflow-owner=WORKFLOWOWNER
  [--workflow-job-owner=WORKFLOWJOBOWNER]
  [--workflow-args="key1:value1 key2:value2 ..."]
  ]
  [--skip-plugins=SKIPPLUGINS]
  [--type=TYPE]
  [--description=DESCRIPTION]
  [--start-date=STARTDATE]
  [--end-date=ENDDATE]
  [--users=USERS]
  [--esaf-id=ESAFID]
  [--proposal-id=PROPOSALID]
  [--run=RUNNAME]
  [key1:value1, key2:value2, ...]
    
```

Description:
 Run DAQ for experiment on station 6BM. If experiment does not exist, it will be added to the DM database. If list of users or proposal id is specified, this command will also add roles for all users listed on the proposal.

globus | Manage Data | Publish | Groups | Support | Account

Transfer Files | Activity | Endpoints | Bookmarks | Console

Endpoint: appsdata | Path: /gdata/ | Go

select all | up one folder | refresh list | share

- 110B Folder
- 110C Folder
- 178M Folder
- 303 Folder
- 3D Folder
- 50D Folder
- 50S Folder
- 50C Folder
- 50D Folder
- 50E Folder
- 50F Folder
- 50G Folder
- 50H Folder
- 50I Folder
- 50J Folder
- 50K Folder
- 50L Folder
- 50M Folder
- 50N Folder
- 50O Folder
- 50P Folder
- 50Q Folder
- 50R Folder
- 50S Folder
- 50T Folder
- 50U Folder
- 50V Folder
- 50W Folder
- 50X Folder
- 50Y Folder
- 50Z Folder
- 50AA Folder
- 50AB Folder
- 50AC Folder
- 50AD Folder
- 50AE Folder
- 50AF Folder
- 50AG Folder
- 50AH Folder
- 50AI Folder
- 50AJ Folder
- 50AK Folder
- 50AL Folder
- 50AM Folder
- 50AN Folder
- 50AO Folder
- 50AP Folder
- 50AQ Folder
- 50AR Folder
- 50AS Folder
- 50AT Folder
- 50AU Folder
- 50AV Folder
- 50AW Folder
- 50AX Folder
- 50AY Folder
- 50AZ Folder
- 50BA Folder
- 50BB Folder
- 50BC Folder
- 50BD Folder
- 50BE Folder
- 50BF Folder
- 50BG Folder
- 50BH Folder
- 50BI Folder
- 50BJ Folder
- 50BK Folder
- 50BL Folder
- 50BM Folder
- 50BN Folder
- 50BO Folder
- 50BP Folder
- 50BQ Folder
- 50BR Folder
- 50BS Folder
- 50BT Folder
- 50BU Folder
- 50BV Folder
- 50BW Folder
- 50BX Folder
- 50BY Folder
- 50BZ Folder
- 50CA Folder
- 50CB Folder
- 50CC Folder
- 50CD Folder
- 50CE Folder
- 50CF Folder
- 50CG Folder
- 50CH Folder
- 50CI Folder
- 50CJ Folder
- 50CK Folder
- 50CL Folder
- 50CM Folder
- 50CN Folder
- 50CO Folder
- 50CP Folder
- 50CQ Folder
- 50CR Folder
- 50CS Folder
- 50CT Folder
- 50CU Folder
- 50CV Folder
- 50CW Folder
- 50CX Folder
- 50CY Folder
- 50CZ Folder
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- 50DH Folder
- 50DI Folder
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- 50DL Folder
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- 50DO Folder
- 50DP Folder
- 50DQ Folder
- 50DR Folder
- 50DS Folder
- 50DT Folder
- 50DU Folder
- 50DV Folder
- 50DW Folder
- 50DX Folder
- 50DY Folder
- 50DZ Folder
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- 50GJ Folder
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- 50GP Folder
- 50GQ Folder
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- 50GS Folder
- 50GT Folder
- 50GU Folder
- 50GV Folder
- 50GW Folder
- 50GX Folder
- 50GY Folder
- 50GZ Folder
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- 50HD Folder
- 50HE Folder
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- 50HG Folder
- 50HH Folder
- 50HI Folder
- 50HJ Folder
- 50HK Folder
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- 50HM Folder
- 50HN Folder
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- 50HS Folder
- 50HT Folder
- 50HU Folder
- 50HV Folder
- 50HW Folder
- 50HX Folder
- 50HY Folder
- 50HZ Folder
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- 50ID Folder
- 50IE Folder
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- 50IJ Folder
- 50IK Folder
- 50IL Folder
- 50IM Folder
- 50IN Folder
- 50IO Folder
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- 50IR Folder
- 50IS Folder
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- 50IU Folder
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- 50IW Folder
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- 50JE Folder
- 50JF Folder
- 50JG Folder
- 50JH Folder
- 50JI Folder
- 50JJ Folder
- 50JK Folder
- 50JL Folder
- 50JM Folder
- 50JN Folder
- 50JO Folder
- 50JP Folder
- 50JQ Folder
- 50JR Folder
- 50JS Folder
- 50JT Folder
- 50JU Folder
- 50JV Folder
- 50JW Folder
- 50JX Folder
- 50JY Folder
- 50JZ Folder
- 50KA Folder
- 50KB Folder
- 50KC Folder
- 50KD Folder
- 50KE Folder
- 50KF Folder
- 50KG Folder
- 50KH Folder
- 50KI Folder
- 50KJ Folder
- 50KK Folder
- 50KL Folder
- 50KM Folder
- 50KN Folder
- 50KO Folder
- 50KP Folder
- 50KQ Folder
- 50KR Folder
- 50KS Folder
- 50KT Folder
- 50KU Folder
- 50KV Folder
- 50KW Folder
- 50KX Folder
- 50KY Folder
- 50KZ Folder
- 50LA Folder
- 50LB Folder
- 50LC Folder
- 50LD Folder
- 50LE Folder
- 50LF Folder
- 50LG Folder
- 50LH Folder
- 50LI Folder
- 50LJ Folder
- 50LK Folder
- 50LL Folder
- 50LM Folder
- 50LN Folder
- 50LO Folder
- 50LP Folder
- 50LQ Folder
- 50LR Folder
- 50LS Folder
- 50LT Folder
- 50LU Folder
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- 50LW Folder
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- 50OJ Folder
- 50OK Folder
- 50OL Folder
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- 50OS Folder
- 50OT Folder
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- 50OW Folder
- 50OX Folder
- 50OY Folder
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- 50PC Folder
- 50PD Folder
- 50PE Folder
- 50PF Folder
- 50PG Folder
- 50PH Folder
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Label This Transfer

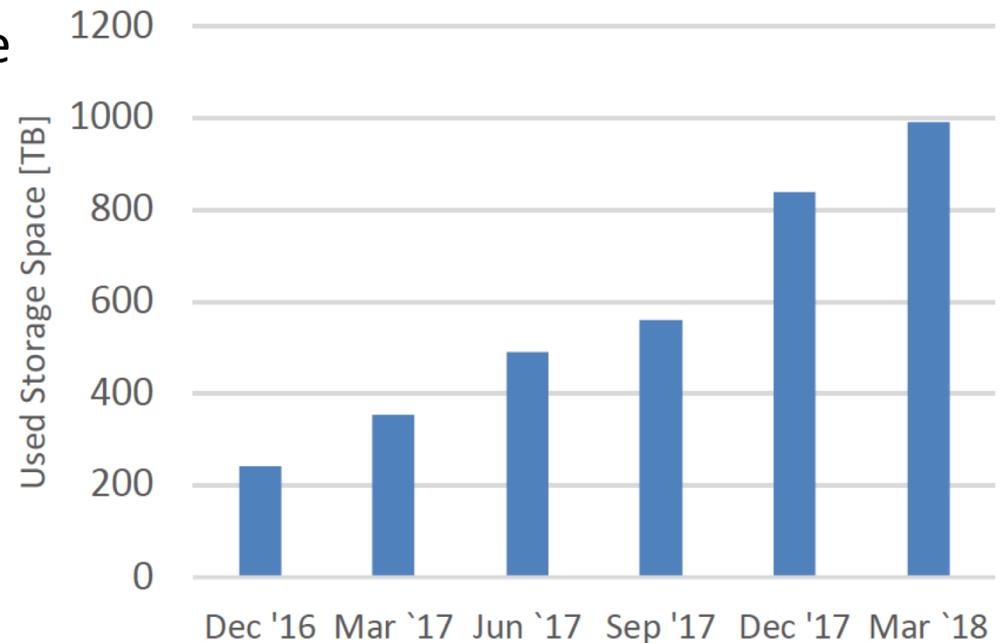
Transfer Settings

- sync - only transfer new or changed files
- delete files on destination that do not exist on source
- preserve source file modification times
- verify file integrity after transfer
- encrypt transfer

System Usage

- December 2016: 5 beamline deployments, 250TB of storage space used
- March 2018: 21 beamline deployments, close to 1PB of storage space used
- Three month average growth of storage space used: 75TB/month

APS Storage Usage



- We are currently using more than 75% of available storage space
- Assuming 75TB/month increase, we have 3-4 months before we run out of space



System Usage: Processing @ 8-ID-I (S. Narayanan)

- 8IDI uses X-ray Photon Correlation Spectroscopy technique (XPCS) for the studies of equilibrium fluctuations and fluctuations about the evolution to equilibrium in condensed matter in the Small-Angle X-ray Scattering (SAXS) geometry
- SPEC software is used for instrument control and data acquisition
- For every raw data file SPEC scripts can start DM processing job based on one of the implemented workflows
- Batch processing workflow:
 - 1) Run a custom shell script to prepare processing environment.
 - 2) Copy raw data file to APS HPC cluster using GridFTP (the *globus-url-copy* command).
 - 3) Append XPCS metadata to the data file by running a custom 8-ID-I utility.
 - 4) Submit a processing job to the SGE batch scheduler via the *qsub* command. This job runs a custom 8-ID-I processing executable.
 - 5) Monitor batch job by running a shell script that interacts with SGE via the *qacct* command.
 - 6) Copy resulting output file into designated beamline storage area using GridFTP (the *globus-url-copy* command).
- Jobs are monitored via static web pages generated by a cron job running DM utilities



Future Plans

- Develop Data Acquisition Service plugins that handle integration with external cataloging and data publishing systems (DOE Data Explorer, Materials Data Facility)
- Storage hardware replacement (purchase approved recently)
- Enable beamline managers to organize their experiment data in storage in a manner that best fits their beamline
- Further develop functionality offered in the DM Station GUI:
 - Improve file metadata and collection views
 - Add workflow and processing job management capabilities
- Enhance DM system monitoring infrastructure:
 - Develop service capabilities for self-diagnosing error or warning conditions and issuing alarms.
 - Improve support for measuring performance (e.g., data transfer rates, file processing rates, etc.)
- Further develop beamline management functionality available in the DM Web Portal
- Develop standard set of workflow definitions that can be reused on different beamlines for automating processing pipelines (need use cases)
- Develop policy engine for automated management of experiment data in storage, archiving of old data, etc.
- Improve documentation, write user guide
- New beamline deployments?
- Archival system?



Conclusions

- The DM system has grown significantly over the last couple of years, in terms of both its usage and capabilities
- The software can be customized and extended to serve individual beamline needs related to data management
- In particular, it can be used to fully automate data acquisition and processing pipelines

Acknowledgements

- APS IT group (R. Sersted and D. Wallis) for their work on building and maintaining the APS On-site Storage and virtual machines used to host beamline DM services
- APS IS group (F. Lacap and Y. Huang) for their help and cooperation with accessing APS databases
- APS SDM group (B. Frosik and A. Glowacki) for many useful discussions
- APS 1-ID (J.-S. Park and P. Kenesei) and 8-ID-I (S. Narayanan) beamlines for their patience, support and help with system testing and troubleshooting since the early prototype versions.
- All DM users



Additional Slides



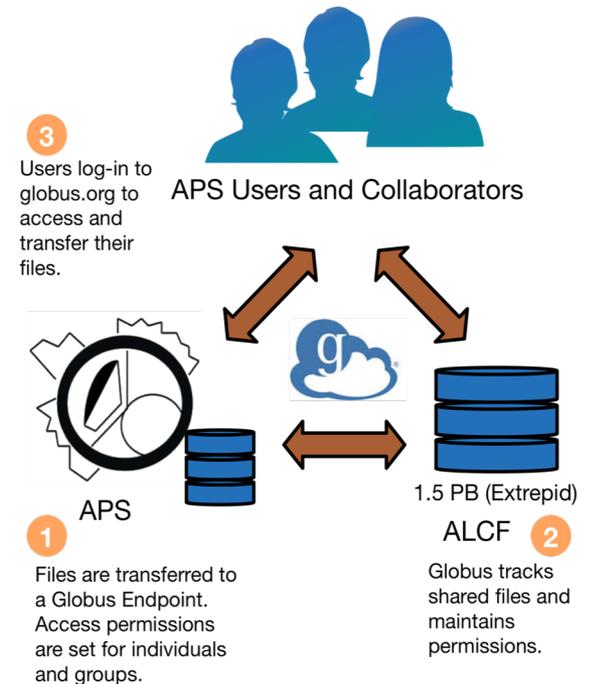
Data Management Challenges?

- How do we organize data?
- Where do we store data?
- How do we store data?
- Do we store all data?
- How do we find data?
- How do we access data?
- How do we manage stored data?
- How can we ensure data integrity?
- Can we automate data acquisition and processing pipelines?
- What can we do about user data analysis and processing?
- ...



A Bit Of History

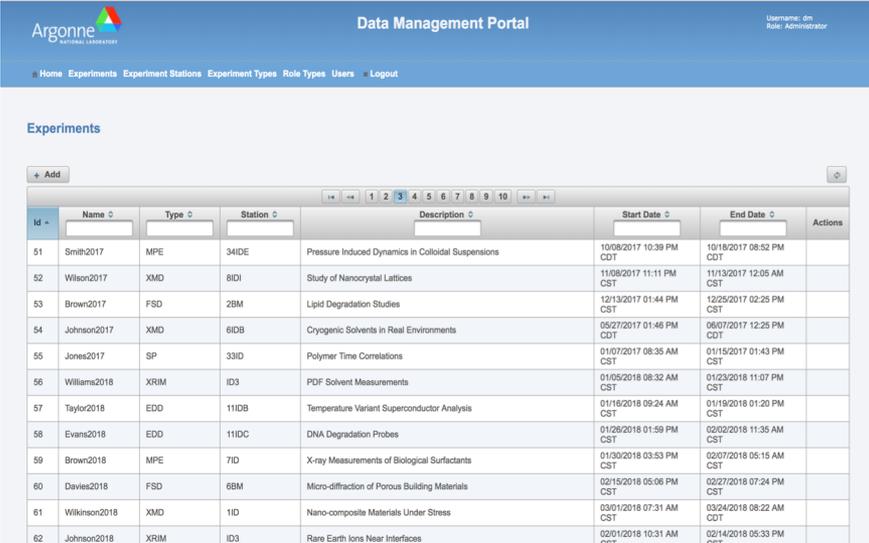
- 2013: Tao Fusion project (LDRD) acquired XSTOR storage (250 TB)
- September 2014: APS Data Management project started
 - Goal: provide APS users with means to easily access their data remotely using Globus Online
- October 2015: First successful software deployment at 6IDD (D. Robinson)



- January 2017: Transition to DDN storage (1.5PB) with high-performance GPFS file system, data redundancy, and 2x10Gbps network links
- March 2018: New VM cluster used exclusively for DM virtual machines
 - Total of 512GB RAM, 144 CPU cores (72x2 due to hyper-threading), 2x10Gbps network links

Site Services

- DM Database (PostgreSQL)
 - Maintains information about users, experiments, and beamline deployments
- Storage Management Service (Python, CherryPy, SQLAlchemy)
 - Runs on the storage head node
 - Provides experiment management services (via REST interfaces)
 - Interacts with LDAP and APS Databases
 - Controls storage file system permissions, which enables data access for remote users
- Web Portal (Java EE Application, Glassfish, JPA, JSF, Primefaces)
 - Experiment management
 - Support for beamline deployments
- Automated utilities for synchronizing DM user information with APS User Database



The screenshot shows the Argonne National Laboratory Data Management Portal. The page title is "Data Management Portal" and the user is logged in as "dm Administrator". The main content area is titled "Experiments" and contains a table with the following data:

Id	Name	Type	Station	Description	Start Date	End Date	Actions
51	Smith2017	MPE	34IDE	Pressure Induced Dynamics in Colloidal Suspensions	10/08/2017 10:39 PM CDT	10/18/2017 08:52 PM CDT	
52	Wilson2017	XMD	8IDI	Study of Nanocrystal Lattices	11/06/2017 11:11 PM CST	11/13/2017 12:05 AM CST	
53	Brown2017	FSD	28M	Lipid Degradation Studies	12/13/2017 01:44 PM CST	12/25/2017 02:25 PM CST	
54	Johnson2017	XMD	6IDB	Cryogenic Solvents in Real Environments	05/27/2017 01:48 PM CDT	06/07/2017 12:25 PM CDT	
55	Jones2017	SP	33ID	Polymer Time Correlations	01/07/2017 08:35 AM CST	01/15/2017 01:43 PM CST	
56	Williams2018	XRIM	ID3	PDF Solvent Measurements	01/05/2018 08:32 AM CST	01/23/2018 11:07 PM CST	
57	Taylor2018	EDD	11IDB	Temperature Variant Superconductor Analysis	01/18/2018 09:24 AM CST	01/19/2018 01:20 PM CST	
58	Evans2018	EDD	11IDC	DNA Degradation Probes	01/26/2018 01:59 PM CST	02/02/2018 11:35 AM CST	
59	Brown2018	MPE	7ID	X-ray Measurements of Biological Surfactants	01/30/2018 03:53 PM CST	02/07/2018 05:15 AM CST	
60	Davies2018	FSD	68M	Micro-diffraction of Porous Building Materials	02/15/2018 05:06 PM CST	02/27/2018 07:24 PM CST	
61	Wilkinson2018	XMD	1ID	Nano-composite Materials Under Stress	03/01/2018 07:31 AM CST	03/24/2018 08:22 AM CDT	
62	Johnson2018	XRIM	ID3	Rare Earth Ions Near Interfaces	02/01/2018 10:31 AM CST	02/14/2018 05:33 PM CST	

Station Services

- Each beamline deployment (“DM Station”) includes several Python services accessible via REST interfaces: DAQ Service, Metadata Catalog and Processing Service
- Data Acquisition Service
 - Responsible for data uploads and for monitoring local file storage
 - Customizable, plugin-based processing framework
 - Plugins handle file transfers, metadata cataloging, interaction with other services
- Metadata Catalog (MongoDB)
 - Metadata are arbitrary key/value pairs
 - Each experiment has its own file metadata collection
 - File metadata can be retrieved using command line or API tools, DM Station GUI, or via the Mongo Express application

```
sveseli — ssh bluegill2 — 100x32
dmadmin@sXiddm> dm-get-file-collection-stats --experiment=Smith-Mar18 --display-keys=ALL --display-format=key-per-line
experimentName=Smith-Mar18
stdDevFileSize=21275858.208
queryDict={}
maxFileSize=251666432
minFileSize=14
collectionSize=1.63133244728e+12
averageFileSize=9634554.76451
nFiles=169321

dmadmin@sXiddm> dm-list-experiment-files --experiment=Smith-Mar18 --display-keys=experimentFilePath,
experimentFileSum
experimentFilePath=pix/macing_000001.tif fileSize=823569 md5Sum=9a87108d6d0bb3bdd16d58b0c7cd6855
experimentFilePath=pix/macing_000002.tif fileSize=823569 md5Sum=7bef341f3625b6db350e4d7060394ca5
experimentFilePath=pix/macing_000003.tif fileSize=823569 md5Sum=ad7399871ce9b4f6dab637d64b2be2fe
experimentFilePath=pix/macing_000004.tif fileSize=823569 md5Sum=d74b11f0438761209e81ac72525cad0
experimentFilePath=pix/macing_000005.tif fileSize=823569 md5Sum=309e7402992ff870f1d0bd7445eb2c39
experimentFilePath=pix/macing_000006.tif fileSize=823569 md5Sum=53e16027b5c2fe3d4ff640c2a847a4ff
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experimentFilePath=pix/macing_000015.tif fileSize=823569 md5Sum=b11a0f65383b795854b5cfca2d79a5af
experimentFilePath=pix/macing_000016.tif fileSize=823569 md5Sum=9bda2ac5161c825d94298d50b0cb817e
dmadmin@s1iddm> |
```

Station Services

- Processing Service provides support for managing user-defined workflows, as well as for submitting and monitoring processing jobs based on those workflows

- DM workflow is a collection of processing steps executed in order:

- Workflow definitions are described as Python dictionaries
- Each processing step must be associated with an (arbitrary) executable
- Support for input/output variables
- Processing steps are automatically parallelized if possible

```
{
  'name': 'tomo-demo-01',
  'description': 'Tomo Demo 01 Workflow',
  'owner': 'pelmer',
  'stages':
  {
    '1-Startup':
    {
      'command': '/home/dm/workflows/tomo-01/start-tomo-01.sh $filePath $outputRootDir',
      'outputVariableRegexList': [
        'Created processing output dir: (?P<outputDir>.*)',
        'File number: (?P<fileNumber>.*)'
      ]
    },
    '2-Process':
    {
      'command': 'ssh txmtwo "source /home/dm/etc/dm.setup.sh > /dev/null;
        /home/dm/workflows/tomo-01/tomo-01.py $filePath $outputDir"'
    },
    '3-Upload':
    {
      'command': 'source /home/dm/etc/dm.setup.sh > /dev/null;
        dm-32id-upload --experiment=$experimentName --data-directory=$outputDir
        --dest-directory=processed/$fileNumber parentFile:$experimentFilePath'
    },
  },
}
```

- Processing Service can be used either standalone, or together with other DM Station services in support of fully automated beamline data acquisition and processing pipelines



Software Installation

- Each beamline at APS has its own Data Management software installation visible to all beamline machines
- Deployment area contains DM software, support software packages, beamline databases, configuration files, various runtime and log files
- All beamlines are fully independent of each other, which works well in the APS environment (beamline machines typically have different maintenance cycles)
- The DM software has fully scripted installation, upgrade, and deployment testing processes, which reduces to a minimum maintenance overhead due to independent beamline software installations
- The DM services typically run on a designated beamline server machine, which can be either virtual or physical (VMs are preferred)
- Services are controlled via a standard set of control scripts suitable for the RHEL operating system used at APS
- Typically, beamline staff has no involvement with DM software installation and maintenance



Support

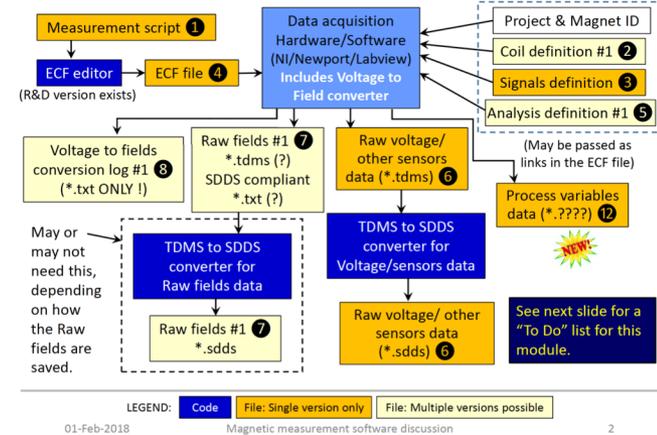
- Official “APS Data Distribution System” support policy:
“Although no guarantees are made as to the system’s availability, problems are addressed as soon as possible on a best-effort basis.”
- Two email lists:
 - DM Users mailing list (dm-users@aps.anl.gov) is used for announcing new software releases, system outages, etc.
 - DM Admin mailing list (dm-admin@aps.anl.gov) can be used for system inquiries



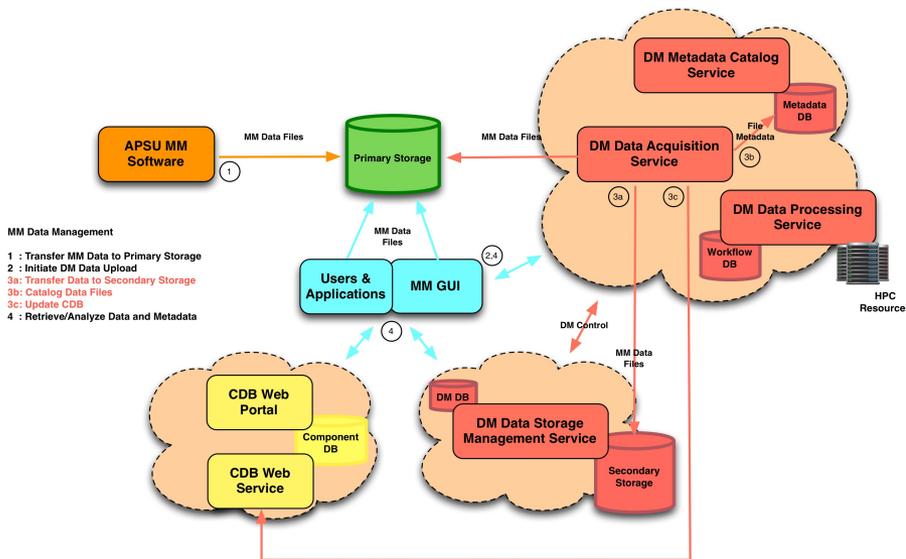
System Usage: APSU MM Data (A. Jain)

- APSU uses Component Database (CDB) for identifying and tracking components needed to build the new facility
- APSU Magnetic Measurements (MM) software works with and creates many different types of files: various definition/configuration files, measurement and analysis files, scripts, raw measurement data, PV data, processed data, log files,...
- Over 1K magnets, each will require multiple measurements => MM software will generate large amounts of data and numerous data files

Overview (Rev 1): Data Acquisition Module



APSU MM Data Management



- DM data upload tools will associate MM experiment with corresponding magnet QR ID in CDB
- During the DM data upload, each MM data file will be processed as follows:
 - Metadata plugin stores file metadata in the APSU DM metadata database
 - CDB plugin adds file item to CDB, and also adds file metadata as item's property
- After the DM data upload, MM experiment item views on the CDB web portal contain links to corresponding magnet, allow downloading experiment files, etc. (CDB work: D. Jarosz)