

Diamond Proposal Manager - v2.2.0

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DuoDesk Proposal Number Find

Id	Ref	Title	Access Route	Last Saved	Status	Action
504412	7067	Default Rapid Access Proposal for I11	Rapid Access	10:40:32, 22 Mar 2011	Submitted	View Edit Copy Remove Submit
504421		Quantitative studies of nanocrystals: determination of local strain, overall shape and their mutual dynamics from a phase-retrieval method applied to combined Bragg and Fraunhofer diffraction data.	Direct Access - New	00:26:43, 22 Mar 2011	Draft	View Edit Copy Remove Submit
504378		Synthesis of New High Density Carbon Phosphide Materials	Direct Access - New	15:57:09, 21 Mar 2011	Draft	View Edit Copy Remove Submit
504419	6683	University of Glasgow/Beatson Institute BAG (Allocation 2)	Programme Mode	15:12:06, 21 Mar 2011	Draft	View Edit Copy Remove Submit
504410		CARENA XAS	Direct Access - New	14:25:50, 21 Mar 2011	Draft	View Edit Copy Remove Submit
504415	7066	Soft X-Ray Resonant Scattering Investigation of Magnetite Thin Films	Direct Access - New	14:06:10, 21 Mar 2011	Submitted	View Edit Copy Remove Submit
504416	6641	BAG Structure of proteins and nucleic acids (Allocation 2)	Programme Mode	14:02:47, 21 Mar 2011	Draft	View Edit Copy Remove Submit
504414		Microfocus XRD studies on the interfacial area between diamonds and metal matrices in diamond tools	Direct Access - Resubmission	14:01:13, 21 Mar 2011	Draft	View Edit Copy Remove Submit
504411		CARENA XRD	Direct Access - New	13:30:21, 21 Mar 2011	Draft	View Edit Copy Remove Submit
504384	7065	FTIR studies on water soluble silicon nanoparticles	Direct Access - New	13:26:21, 21 Mar 2011	Submitted	View Edit Copy Remove Submit

Submit Proposal

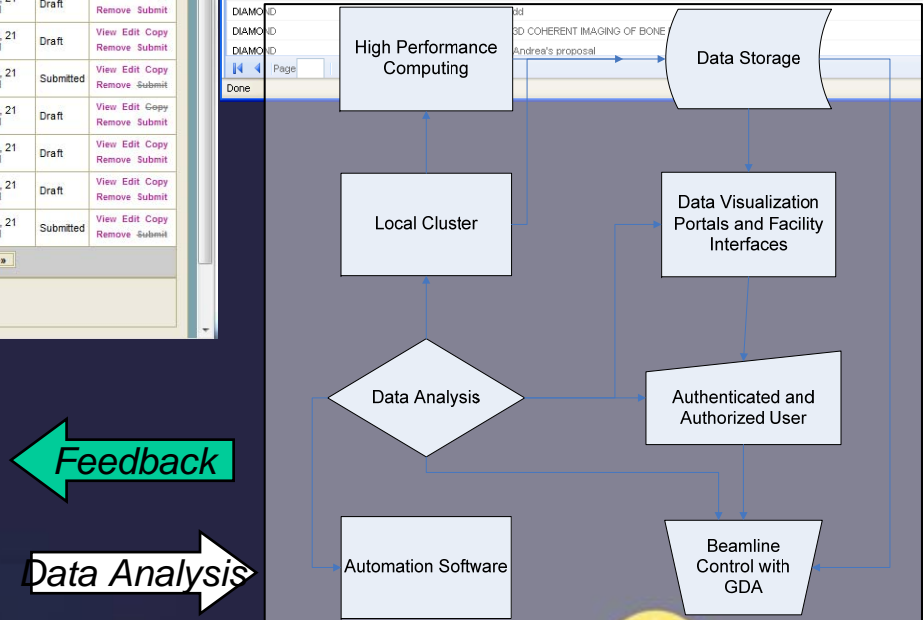
TOPCAT web tool for multiple iCAT services - Mozilla Firefox

Science & Technology Facilities Council

My Data

Facility Name	Investigation Number	Title	Start Date	End Date
DIAMOND	SW19	G12 making		
DIAMOND	SW19	G12 making		
DIAMOND	SW19	G12 making		
DIAMOND	NT149	test5		
DIAMOND	SW19	G12 making		
DIAMOND	NT1872	Andrea's proposal		
DIAMOND	NT1872	Andrea's proposal		
DIAMOND	NT1872	Andrea's proposal		
DIAMOND	SP2042	MX testing Proposal		
DIAMOND	MX1978	Generalized testing Proposal		
DIAMOND	SW19	G12 making		
DIAMOND	SW19	G12 making		
DIAMOND	SP426	Data pipeline tests on I06		
DIAMOND	SP429	Data pipeline tests on I18		

Results



Feedback

Data Analysis

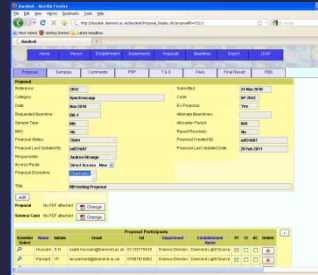
Excited Users



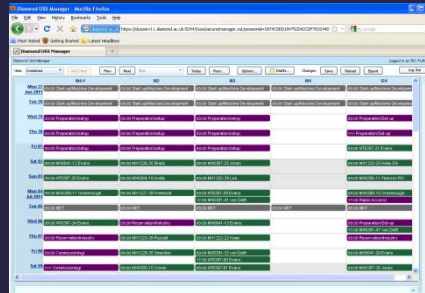
The process



Proposal Submission
duo.diamond.ac.uk

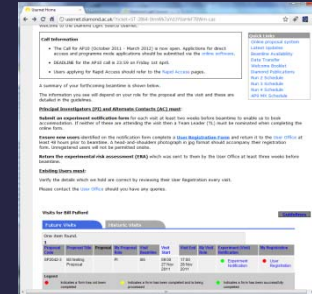


duodesk.diamond.ac.uk

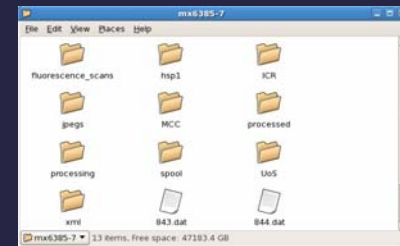


Scheduling
uss.diamond.ac.uk

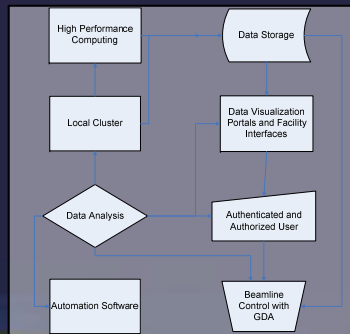
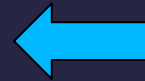
*Currently 5749 Visits for MX
7,000,000 files/~93Tb*



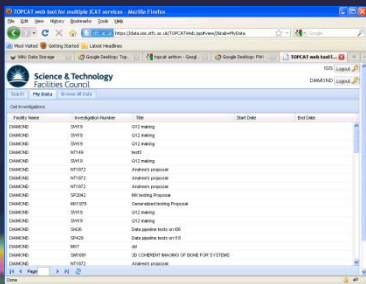
User Interaction
usernet.diamond.ac.uk



Create Directories



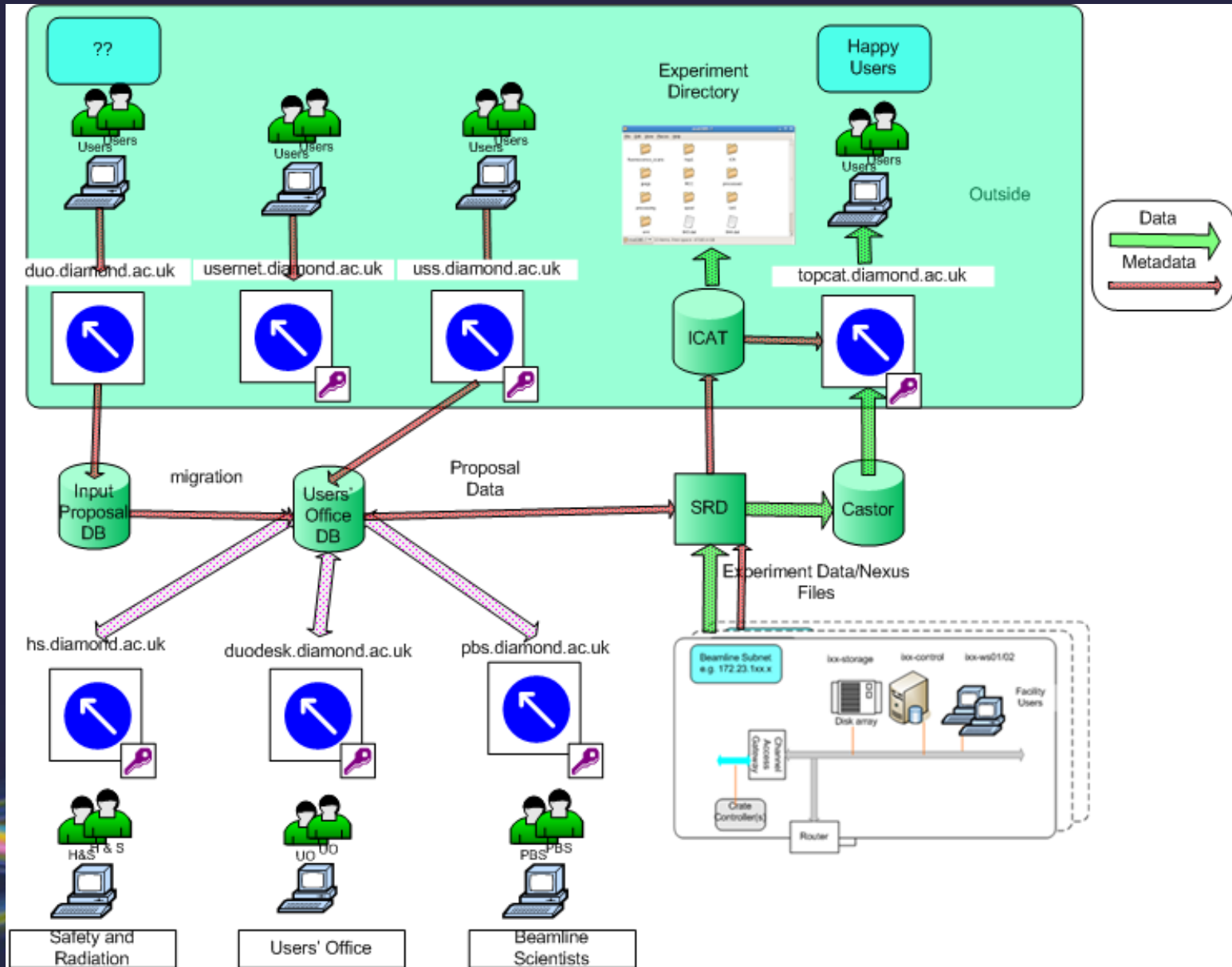
Acquisition/Analysis



Data Portal
topcat.diamond.ac.uk



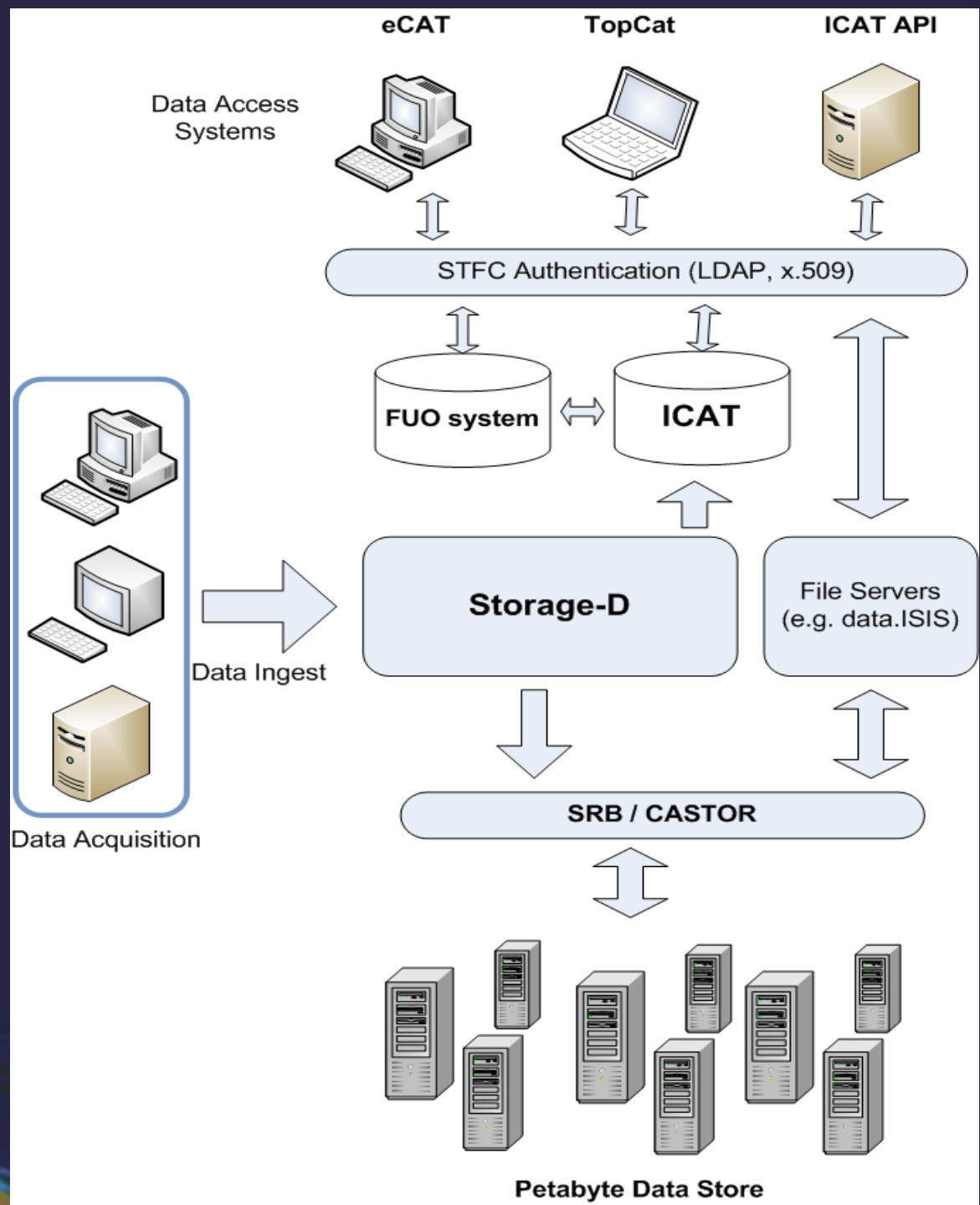
Current Position



Experimental Data Flow

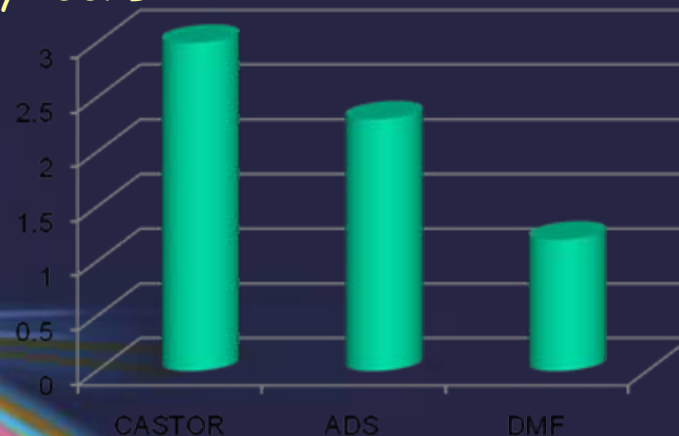
A Common set of Components

- Independent components
- Which can interface to each other.
- Can be adopted and adapted into different situations, and different services



Current State: Diverse Data Storage and Management Technologies

- Tape Libraries:
 - 2 x SD8500 10,000 slot robots
 - 64 tape drives
 - 9940B (0.2 TB)
 - T10KA (0.5 TB, ~ £200K/PB)
 - T10KB (1 TB, ~ £100K/PB)
 - T10KC (5TB, ~ £30K/PB)
 - Total of ~ 7PB tape storage
 - Potential capacity 100PB
- Data management and archive systems:
 - CASTOR (HSM, ORACLE, Scalable, Tier-1)
 - DMF (HSM, NFS access via LAN)
 - Atlas Data Store (Dark Archive)



“User” Technologies
Storage-D
Storage Resource Broker
I-RODS
Storage Resource Manager
ICAT
Top CAT

Topcat

The screenshot shows a web browser window with the URL <https://data.isis.stfc.ac.uk/TOPCATWeb.jsp#view//&tab=AllData>. The page header includes the Science & Technology Facilities Council logo and navigation links for 'Search', 'My Data', and 'Browse All Data'. User accounts for 'ISIS' and 'DIAMOND' are visible in the top right corner.

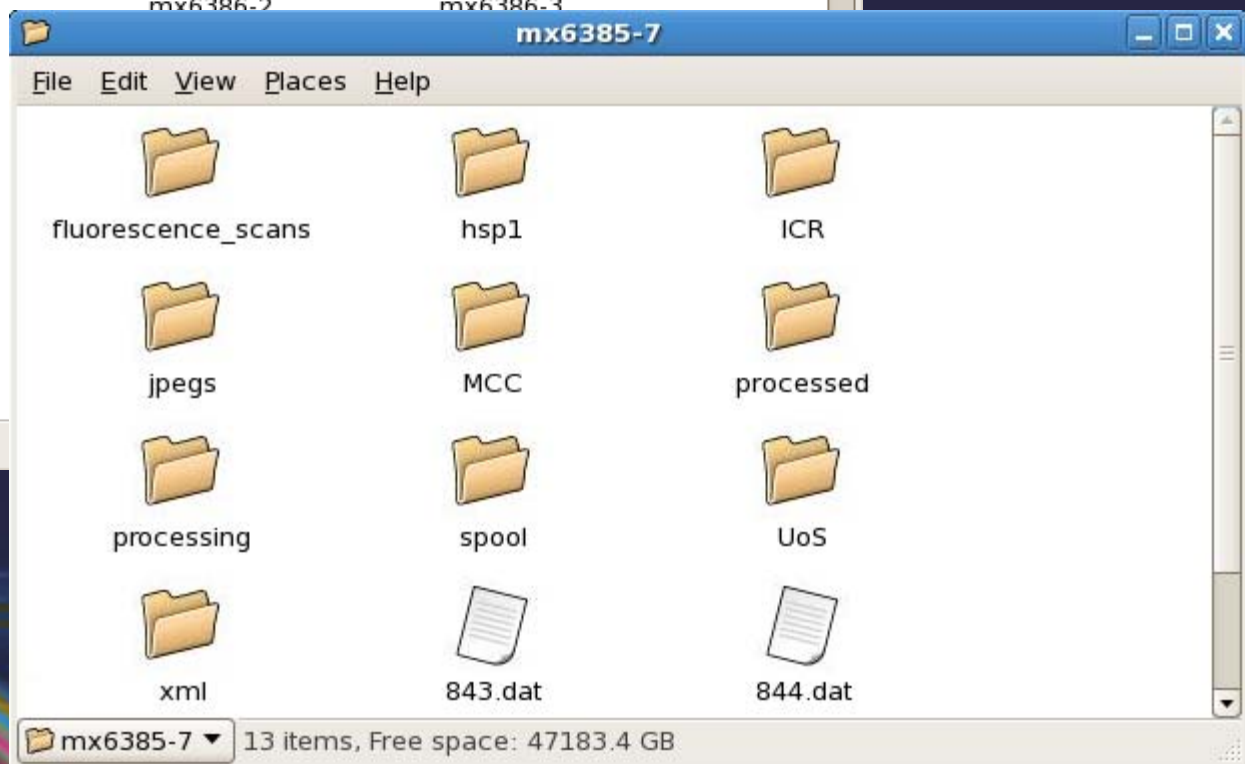
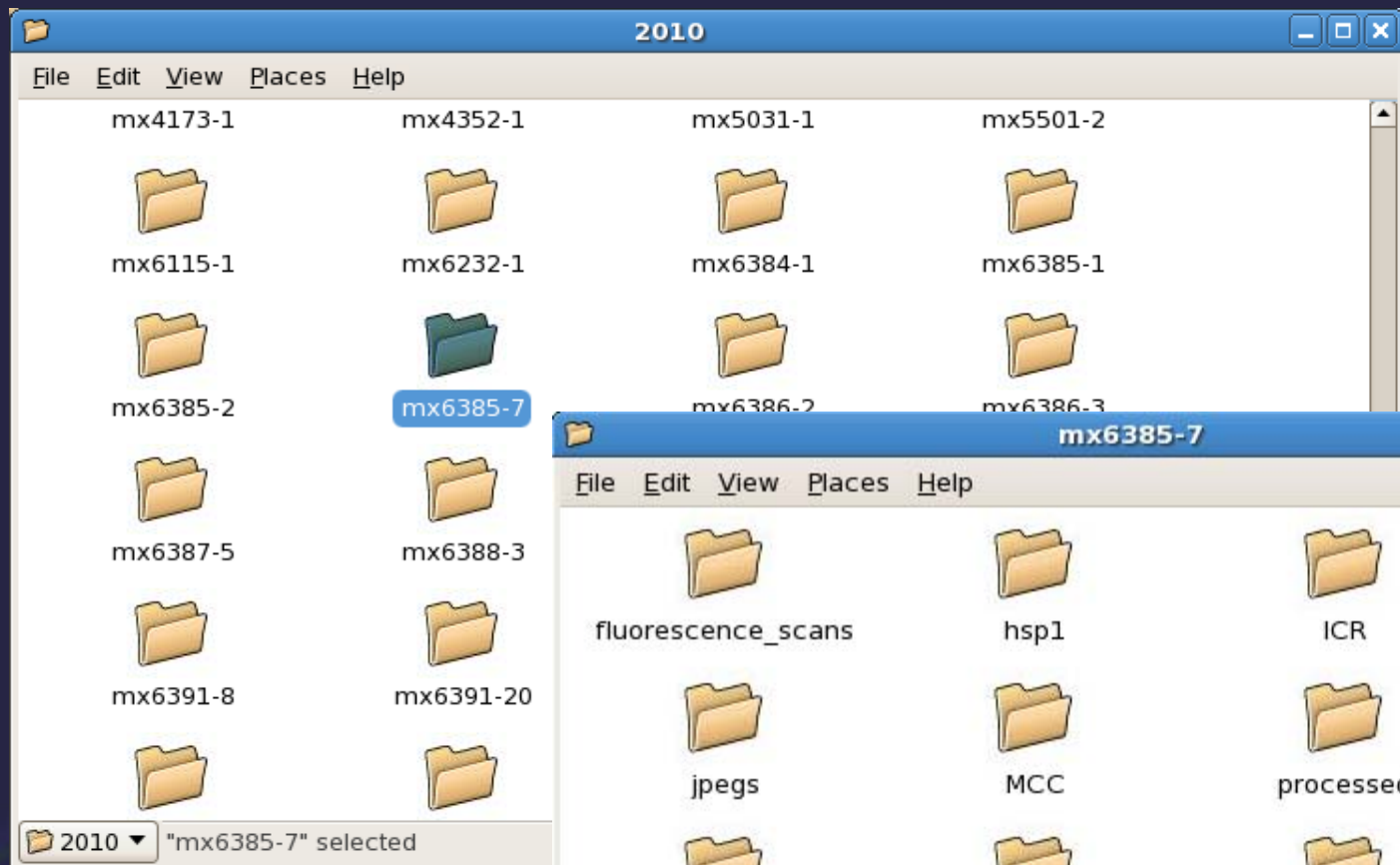
The main content area displays a hierarchical file tree:

- Download
- ISIS
- DIAMOND
 - any
 - b16
 - b18
 - b21
 - b22
 - Spectroscopy of microporous single crystals(id:CD3011)
 - AIPO5
 - Co STA15
 - Co-STA-15 LP-110 as prep no pol on ZnSe crystal2 1024.0
 - Cu-MgAPO-STA-6
 - Cu-SAPO-STA7
 - DAF-1
 - Fe-STA15
 - Friday after lunch
 - MgALPO-5
 - MgAlPO4-5 pol0 crystal1.0
 - MgAlPO4-5 pol0 crystal2 horiz.0
 - MgAlPO4-5 pol0 crystal3.0
 - MgAlPO4-5 pol90 crystal1.0
 - MgAlPO4-5 pol90 crystal3.0
 - MgAlPO4-5 without pol crystal1.0
 - MgAlPO4-5 without pol crystal2 horiz.0
 - MgAlPO4-5 without pol crystal3.0
 - MgSTA-15
 - MgSTA-15 calcined
 - MgSTA15
 - SAPO-STA-6 ZH11

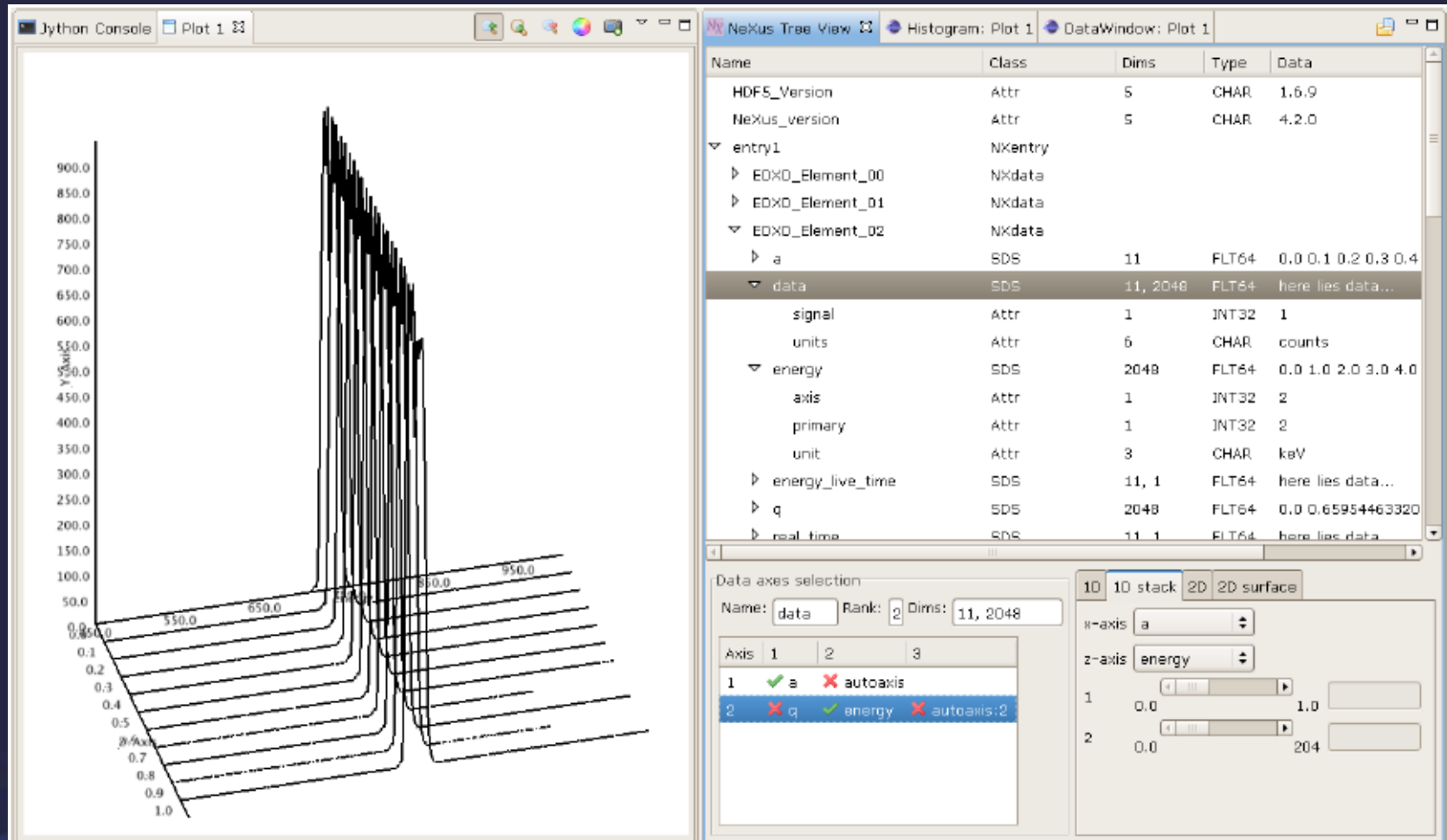
Data Volumes and Numbers of files ~ 147Tb

Beamline	Data Volume (GB)	No. Files	Type
b16	4430.71	428631	Materials
b18	268.71	47180	Spectroscopy
b22	47.84	22212	Infrared
b23	0.2	11439	CD
i02	27460.36	1842753	MX
i03	35580.91	3212342	MX
i04	20593.17	1264886	MX
i04-1	6816.37	1678377	MX
i06	165.24	593404	Nanostructures
i06-1	135.64	91180	Nanostructures
i07	1166.33	479522	Surfaces
i10	0.49	7436	Dichroism
i11	298.66	609614	Powders
i12	22443.83	1286900	Tomography
i15	1215.39	317753	High Pressure
i16	2967.78	2555149	Materials
i18	1288.58	15876367	Spectroscopy
i19	3449.95	1848476	SX
i20	8.78	11986	Spectroscopy
i22	1204.27	317084	NCD
i24	17378.41	259567	MX

Data Directories



Nexus Metadata



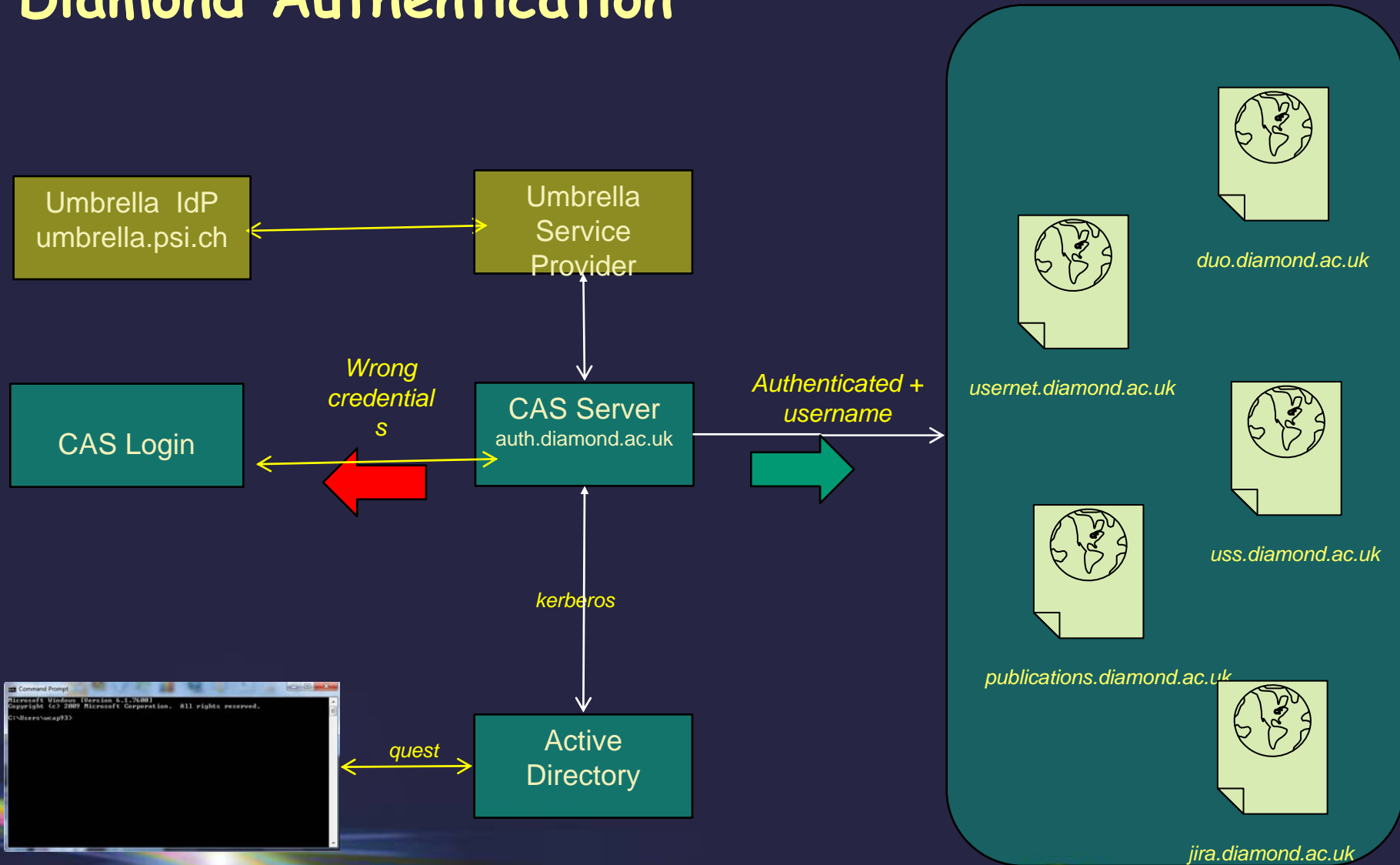
Draft models of Nexus metadata available for Spectroscopy, Non Crystalline Diffraction, Tomography. MX exists



Requirements for cross facility AAA

- The aim of this project is to provide a mechanism for uniquely identifying users of large scientific facilities and associated communities irrespective of their method of access. For the purposes of the report this authenticator would be given the name ESP or European Scientific Pass. (Consider ESI for European Scientific Identifier)
- All users of the major facilities will need only one username/password combination to access any of the facilities.
- The local user administration offices should be the principal controllers of authorisation.
- Users must be able to update their own passwords or other personal data using a "Bank Type" web application.
- The process of gaining a network identifier would require proof of identity but must be accomplished in a few minutes.
- These credentials or an automatically generated certificate or token will allow access to any computing technology given the correct authorization.
- The authorization will be performed locally by the facility involved based on the single unique identifier derived from 1-3.
- The AAA system would extend to scientists and engineers supporting data acquisition and analysis at their facilities. The authentication and authorization implicit in the system provides the necessary access security requested in the outline document.

Diamond Authentication



Interactive session

Planned or foreseen (no promises!)

- The Users may easily expect to see their data in the directory structure above. A FUSE based (probably) interface is planned to enable this. i.e. The directories may be NFS or SMB mounted.
- Longer term a file browser for Linux or Windows may be made available with properties mirroring the ICAT metadata.
- Needed ability to establish interactive sessions in addition to AD. E.g X509 Certificates

Example Use of PANDATA and AAA

- This is the key challenge in that it requires agreement and acceptance from the scientific community. They should see major advantages in subscribing together with a simple and efficient system to put this in effect. Historically grid type solutions using certificates and middleware have proven too heavy and slow for synchrotron users (study done by ESRF).

