

DataFed

A Federated Scientific Data Management System for Reproducible Science

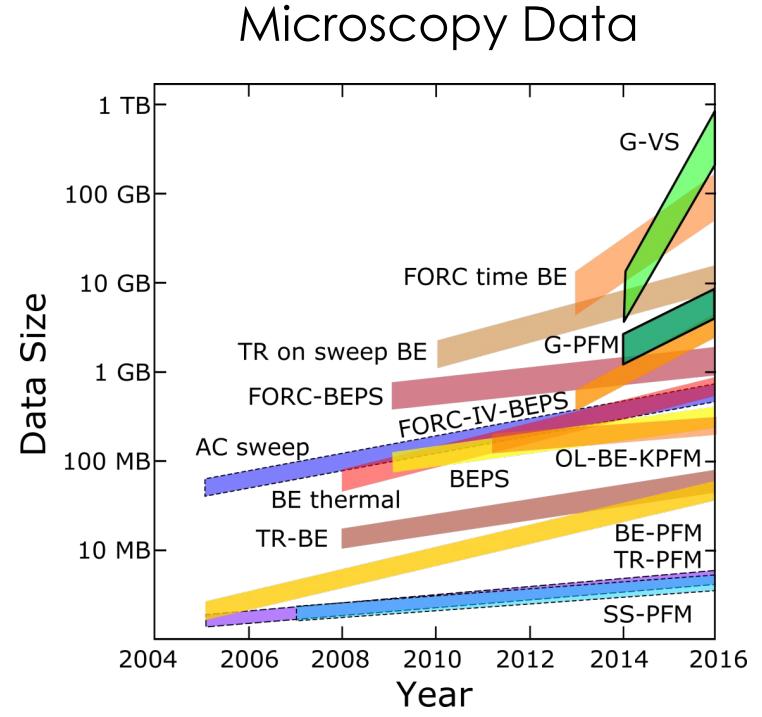
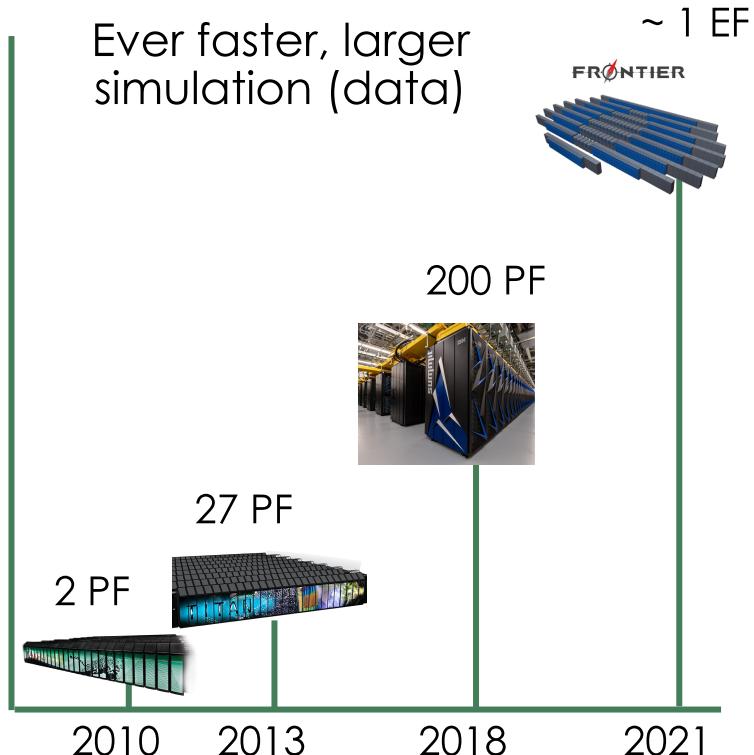
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Advanced Data and Workflows Group
Oak Ridge Leadership Computing Facility

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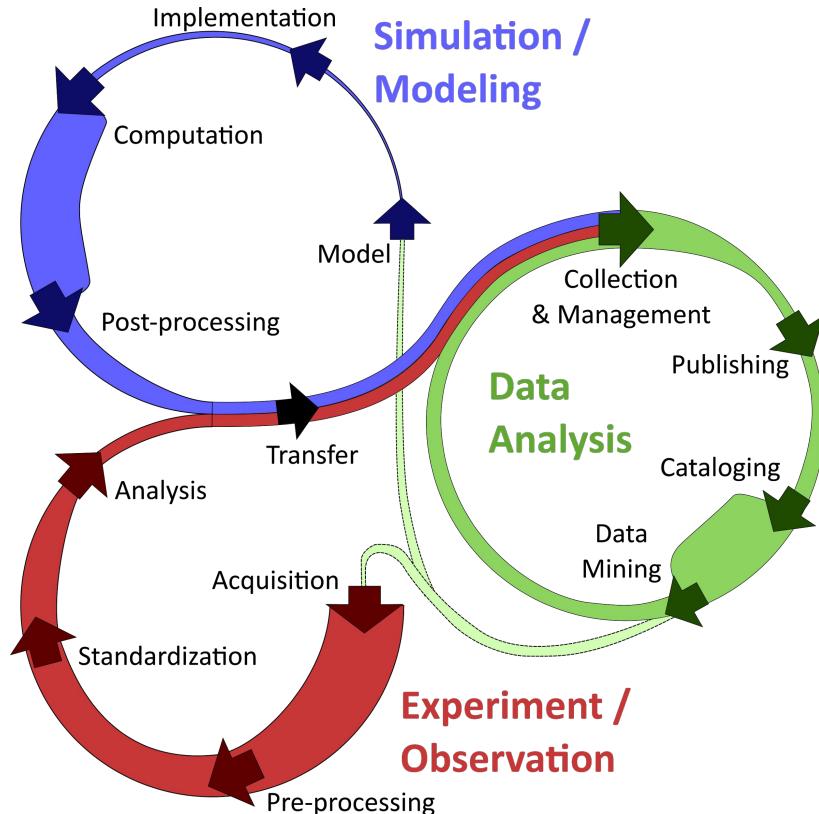


Explosion in Data Volume, not (necessarily) Quality



Kalinin et al., ACS Nano, 9068-9086, 2015

Complex Data Lifecycle



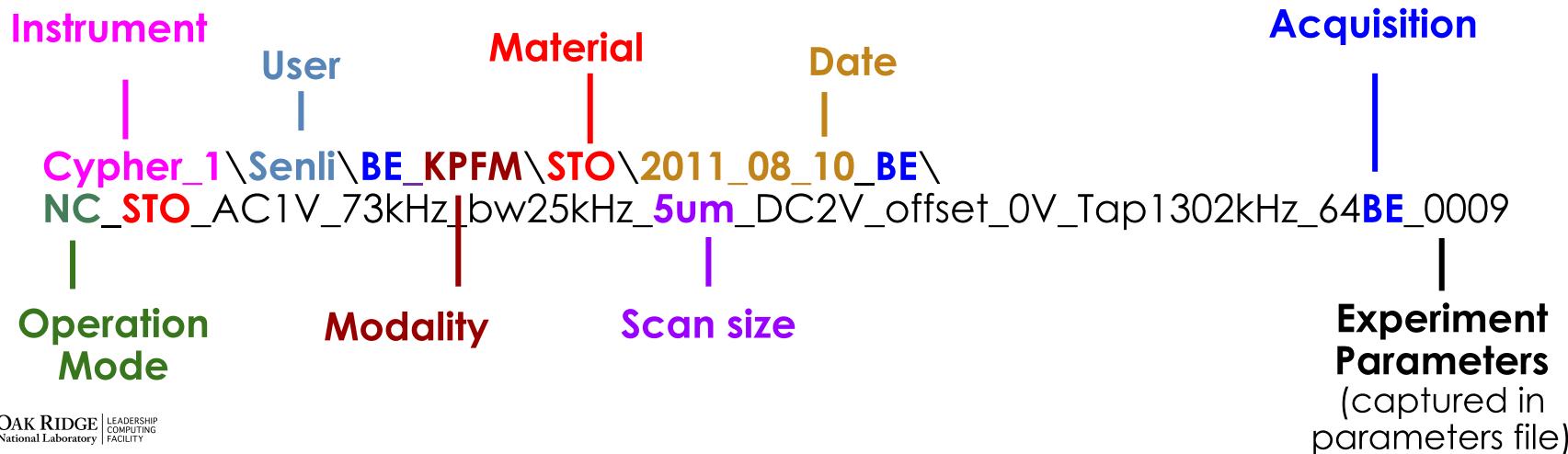
- Interplay of discovery paradigms
- Validation
- Reuse
- Global collaboration

Thickness
=

Data volume

Laborious Wrangling of Unstructured (Meta)data

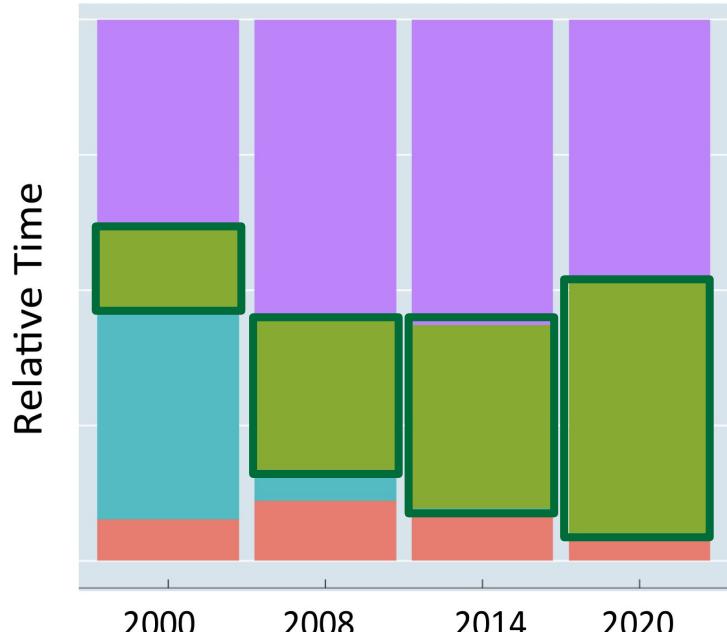
- Various and proprietary file formats
- Relevant metadata rarely available / indexed / searchable
 - Not all metadata may be available
 - Naming and structure varies by user and time
 - Most often embedded in file names



Explosion in Time Spent on Data Management

Experimental Time Breakdown

Experiment Design Management Measurements Post Processing



* at light sources

Need for Scientific Data Management

- Ever more time spent on data management
- Explosion in data generation
 - Data generation rate outstrips consumption rate
 - Opportunities for discovery through analysis
- Scientific research more complex, globalized, collaborative now
- Increased need and pressure to share data
- Reproducibility crisis in science

Scientific Data Management Systems

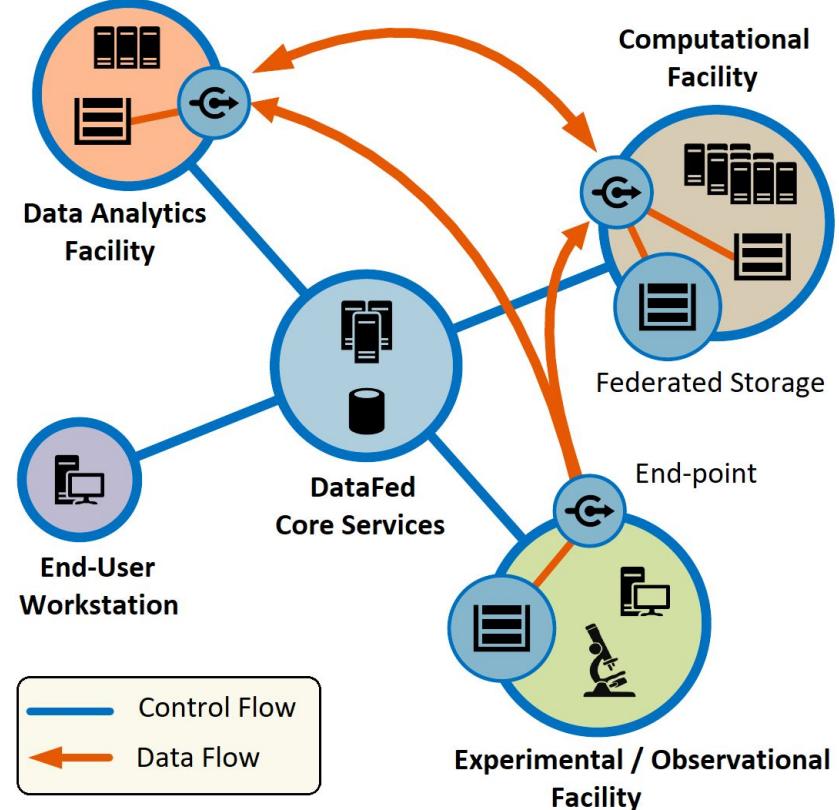
- Data handling application
- Unique identifiers for each record, collection, user, etc.
- Abstracts file system complexities (directories, paths, files,)
- Indexes metadata
 - General - author, creation date, size, provenance, etc.
 - Domain-specific
- Powerful searches
- Collaboration via fine-grained access control

Scientific Data Management Systems Today

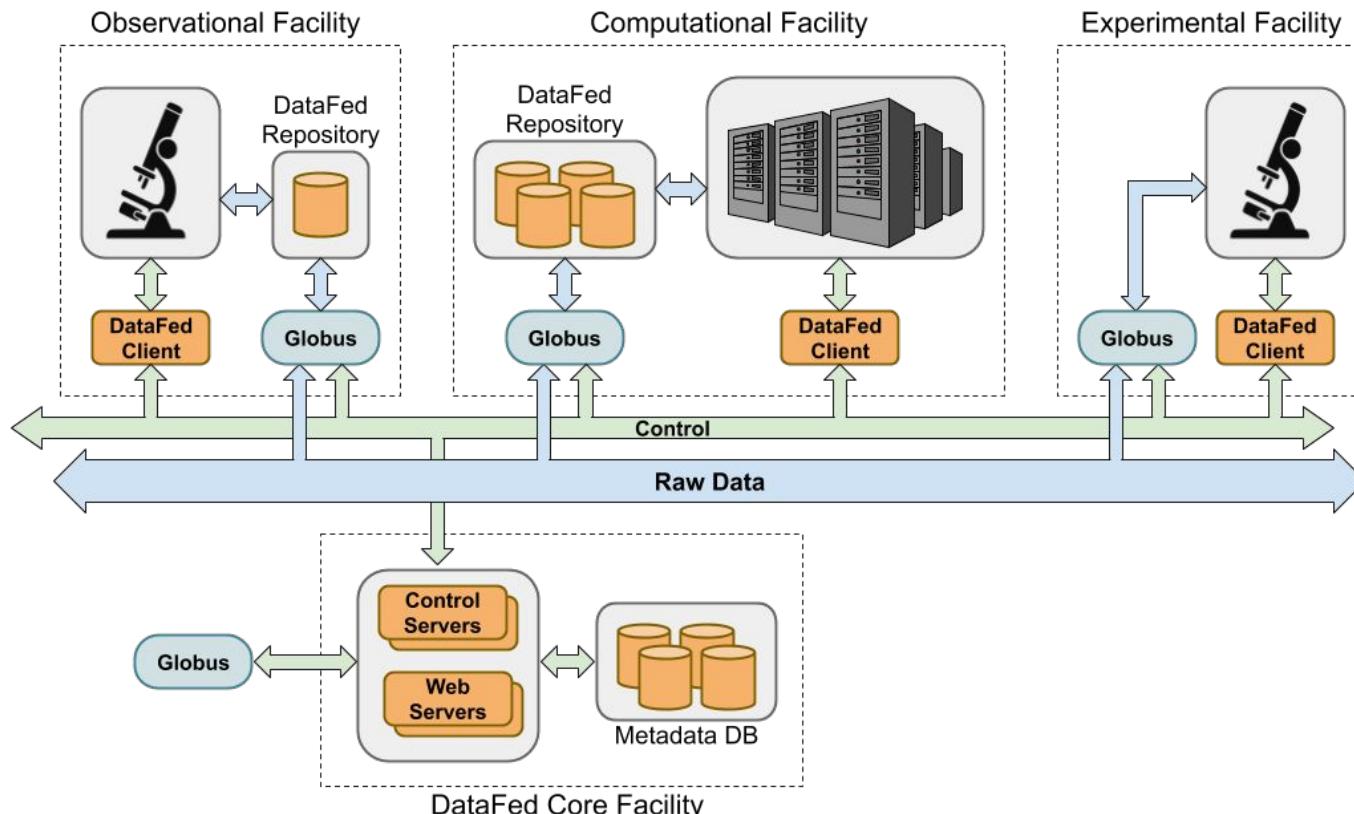
- Regularly used in commercial / production-oriented workflows
 - Highly specific to company / application
- Some used in academia
 - Rucio, iRODS, Clowder, Omero, K-Base, ...
 - Often rigid / tailored to specific scientific domains
 - Often using non-performant / non-scalable:
 - Data transfer - SCP / SFTP
 - Identity management - Virtual organizations

DataFed

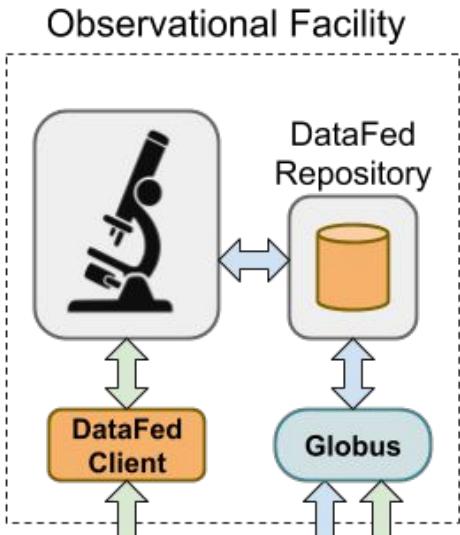
- General purpose, opt-in SDMS
- Federation of data repositories
- Using Globus for:
 - File transfers
 - Federated identity management
- Supports Findable, Accessible, Interoperable, Reusable (FAIR) principles
- Designed with HPC and big data in mind
- Spans facilities and organizations



DataFed - Federation of Data Repositories

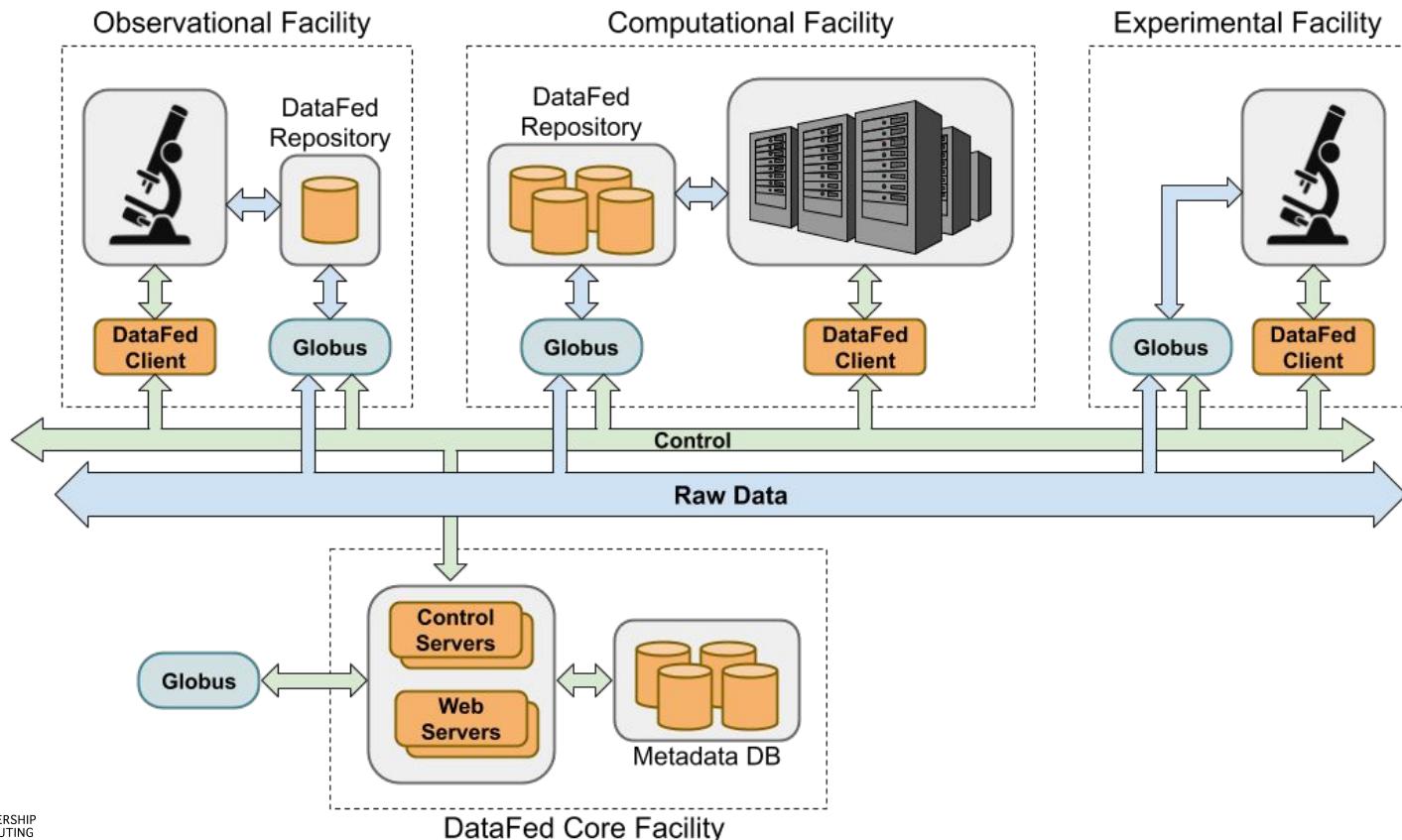


DataFed Repositories

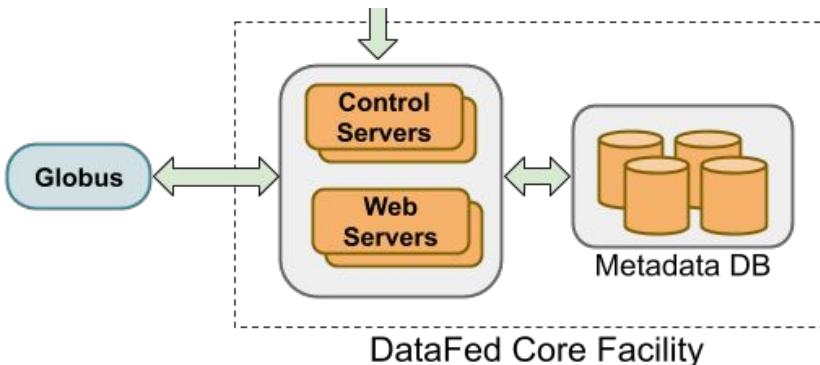


- Connect facility-local data storage to DataFed network via dedicated Globus endpoint
- Any file-system supported by Globus
- DataFed handles authorization, concurrency control, access control, etc.
- Raw binary data stays in repository
 - Managed by DataFed
 - Metadata in DataFed Database servers

DataFed - Federation of Data Repositories



Core Services



- Control Servers
 - Orchestrating activities - data transfers, concurrent data access
 - Gateway to microservices within database
- Web Servers
 - Interface with control servers - Web Portal
- Database
 - Houses metadata for all records
 - State of DataFed network - users, projects, repositories, etc.

DataFed Interfaces - Web Portal and CLI

The screenshot shows the DataFed web interface. On the left, a sidebar navigation includes 'My Data' (selected), Catalogs, Provenance, and Search. Under 'My Data', there are sections for Root Collection, Demo, and My Projects. The 'Demo' section is expanded, showing datasets like 'Calibration Titan 1/1/2019' and 'Config Titan 123'. A specific dataset, 'Dataset A', is selected and detailed in the main pane. The 'Selection Information' panel shows the Data ID (d/67776565) and Alias (data-a). The 'Description' panel contains the text: "An interesting scientific dataset". The 'Dependencies' panel lists it as a component of d/67780272 (exp-1) and a precursor of d/67776773 (data-c). The 'Details' and 'Metadata' panels are also visible.

```
ls
1. c/53987481 (demo)           "Demo"
2. c/51962668 (share)          "Share"
3. c/53986809 (test)          "Test"
>ls demo
1. d/67781402 (cal-titan-010119) "Calibration Titan 1/1/2019"
2. d/67781026 (config-titan-123) "Config Titan 123"
3. d/67776565 (data-a)          "Dataset A"
4. d/67776684 (data-b)          "Dataset B"
5. d/67776768 (data-b-1)        "Dataset B-1"
6. d/67777979 (data-e)          "Dataset E"
7. d/67779849 (data-f)          "Dataset F"
8. d/67776773 (data-c)          "Dataset-C"
9. d/67776892 (data-d)          "Dataset-D"
10. d/67780272 (exp-1)         "Experiment 1"
>dv 3.
DataID  d/67776565 (data-a)
Title   Dataset A
Desc    An interesting scientific dataset
Topic   n/a
Keywords data science, machine learning
Owner   u/stansberrydv
Locked  No
Size    0
Repo    repo/core
Created 2019-04-03 16:28:00
Updated 2019-04-03 16:42:30
Meta    (available)
Refs   Child of d/67780272 (exp-1)
       Source of d/67776773 (data-c)
>^C
[3ub@or-condo-login01 ~]$ exit
logout
Connection to or-condo-login.ornl.gov closed.
(base) persimmon:~ 3ub$
```

Modern web application

Command-line & Python package

Interactive & non-interactive scripting (e.g.
- HPC environments)

General Metadata

The screenshot shows the DataFed v-0.7.2 web application. The top navigation bar includes 'Help' and 'Log Out'. The main menu has tabs for 'My Data', 'Catalogs', and 'Search'. The 'My Data' tab is active, showing a tree view of datasets under 'Root Collection'. A specific dataset, 'VS126No2_BEline_0002', is selected and highlighted with a green border. The 'Selection Information' panel displays the Data ID (d/10337910), Alias ('vs126no2_beline_0002'), and the name of the selected item ('VS126No2_BEline_0002'). The 'Provenance' section indicates 'No relationships.' The 'Details' section provides the following metadata:

Keywords:	pt,lsmo,pto,lsm
Locked:	No
Data Repo:	cades-test
Data Size:	37.6 MB
Source:	57230a10-7ba2-11e7-8c3b-22000b9923ef/lustre/or-hydra/cades-ccsd/syz/pycrosropy_ensemble/be_sho/Nanophase_Done/VS126No2_BEline_0002.h5
Extension:	.h5

Below the details are buttons for 'Provenance', 'Edit', 'Delete', 'Sharing', 'Lock', 'Unlock', 'Get', 'Put', and 'Relocate'. The bottom search and filter bar includes fields for 'ID/Alias', 'Text', 'Metadata', and checkboxes for 'Scope' (My Data, My Projects, Other Projects, Shared, Selected). Buttons for 'Run Query', 'Save Query', and 'Clear Sel.' are also present.

- Owner
- Repo
- Size
- Keywords
- Tags
- Provenance
- Searchable

Domain-Specific Metadata

- Arbitrary tree
- String, numeric, array values
- Searchable
- Support for community defined schemas
- upcoming

The screenshot shows the DataFed v-0.7.2 user interface. The top navigation bar includes tabs for "My Data", "Catalogs", and "Search". The main content area displays a hierarchical file tree under "My Data". A specific folder named "VS126No2_BEline_0002" is selected and highlighted with a green background. Below the tree are several action buttons: Provenance, Edit, Delete, Sharing, Lock, Unlock, Get, Put, and Relocate. At the bottom of the interface, there are search fields for "ID/Alias" and "Text", and a "Metadata:" field marked with an asterisk (*). The "Scope" section at the very bottom allows filtering by "My Data", "My Projects", "Other Projects", "Shared", and "Selected".

Selection Information

- Metadata
 - data
 - file_properties
 - measurement_properties
- source : "Atomic Force Microscope"
- instrument : "Asylum Research Cypher"
- modality : "Band Excitation Scan"
- project
 - investigator_name : "Yunseok"
 - project_id : "Unknown"
 - host_institution : "Center for Nanophase Materials Science"
- sample
 - materials
- O : "Pt"

Metadata

Search

DataFed v-0.7.20

My Data Catalogs Search

- "PZT_cap_line_2um_0004" (pzt_cap_line_2um_0004)
- "PZTcer0005_BElineL_0001" (pztcer0005_belineL_0001)
- "PE60_spot2_5um_1Vac_pm20V..." (pe60_spot2_5um_1vac_pm20v_0001)
- "F186_BEline_0001" (f186_beline_0001)
- "29052016PZTFT4_BE_0002" (29052016pztf4_be_0002)
- "LSATLSMOPZTP1505LAOLSMOP..." (lsatlsmopztp1505laolsmopztp_0001)
- "6October2014PZT3000nm_0004" (6october2014pz3000nm_0004)
- "JA0020_BElineV_after_0001" (ja0020_belinev_after_0001)
- "V181_BEline_0002" (v181_beline_0002)
- "PZT150j0012_BEline_0001" (pzt150j0012_beline_0001)
- "LSATLSMOPZTPLSATLSMOPZTP..." (lsatlsmopztplsatlsmopztp_0001)
- "IT0RZTPBN2800nmVeryGood_B..." (it0rztpbn2800nmverygood_b...)

Selection Information

- file_properties
- measurement_properties:
 - source : "Atomic Force Microscope"
 - instrument : "Asylum Research Cypher"
 - modality : "Band Excitation Scan"
- project
- sample
 - materials
 - 0 : "PZT"
 - thickness_[nm] : 3000
- time
- type
 - data_type : "Spectroscopic Imaging"
 - subject : "Small sample"

Provenance Edit Delete Sharing Lock Unlock Get Put Relocate

Search Transfers Allocations Settings

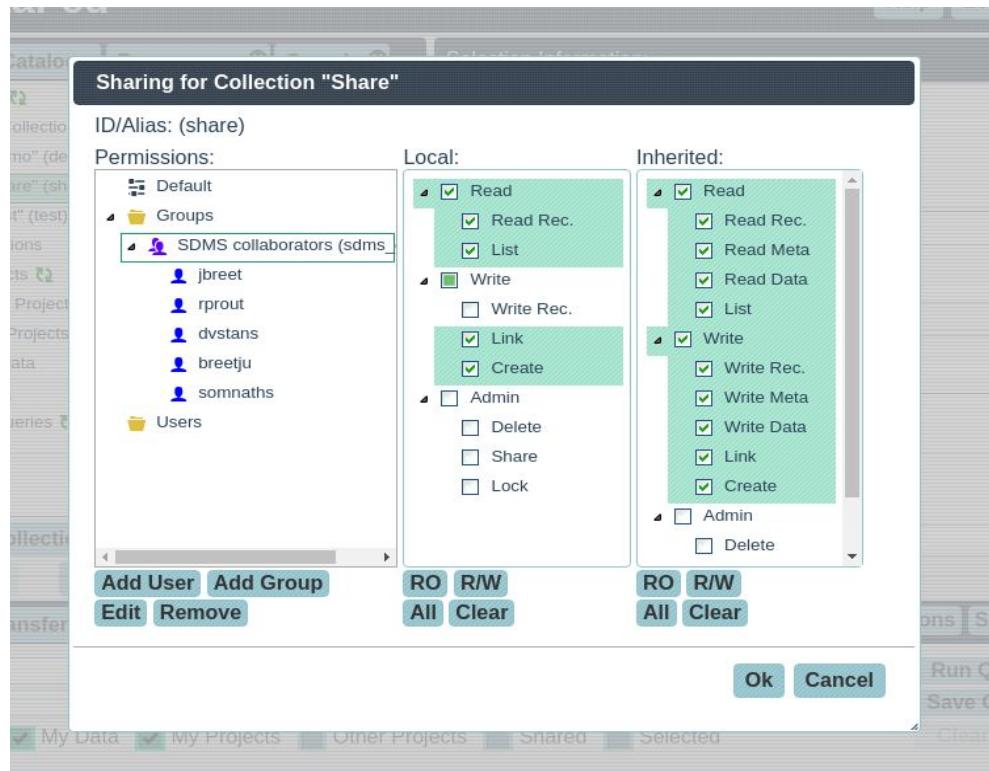
ID/Alias: Text: Run Query

Metadata: * `"PZT" in sample.materials && type.data_type == "Spectroscopic Imaging" && measurement_properties.modality == "Band Excitation Scan"` Save Query

Scope: My Data My Projects Other Projects Shared Selected Clear Sel.

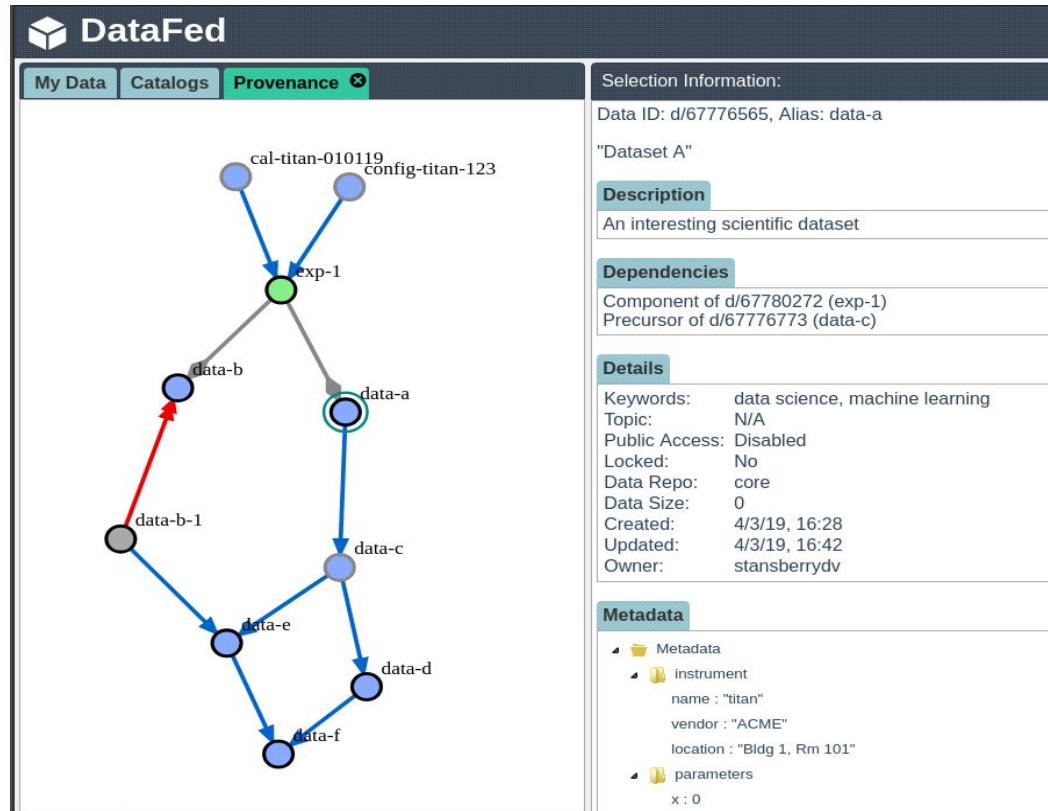
Fine-Grained Access Control

- Per user or group, and default
- Per record, or collection
- Inherited from parent collection(s)
- Differing permissions for records and collections



Provenance Capture

- Currently supports:
 - “Derived from”
 - “Component of”
 - “New version of”
- More coming soon
- User-defined relationships
 - “Calibration associated with”
 - ...



Projects

Catalogs Selection Information:

New Project

ID:	cadescdemo-1
Title:	Demo project
Description:	New project with admin, members, and a sub-allocation on core <u>repo</u> .
Owner:	stansberrydv
Sub-allocation:	core (6.6 MB / 11.4 MB) ▾
Alloc. Size:	1 MB
Members:	breetju rprout shubhankar
Admins:	somnaths

Add Remove Add Remove

Create Cancel

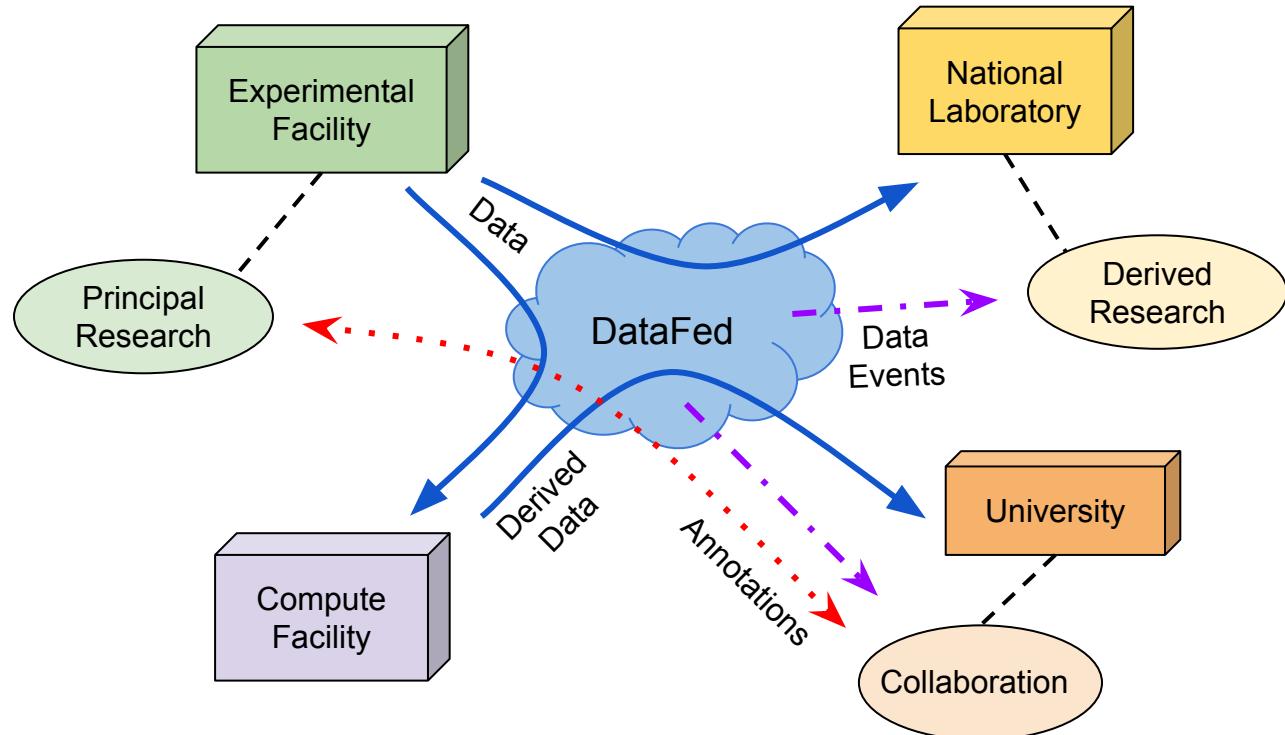
- Collective ownership of data
- Projects similar to user accounts
- Can be created by any user
- Assign admins and members
- Assign repository allocations
- Dedicated collection hierarchy
- Data owned by project
 - Member access based on admin defined permissions

Cross-Facility Collaboration & Derived Research

Publish-subscribe
to data records

Subscribers
notified of
upstream events

Creators notified
about
annotations such
as errors



Other DataFed Features

- Collections of records
- Dynamic views - saved search queries
- Allocations per user, project
- Exploring related data based on provenance graphs, keywords, tags
- Scripting, batch processing and workflow support
- Catalog view of pre-published data - discoverable, explorable
- Scalable administration of repositories
 - Globus handles federated identity management
 - Simple sign-on with Globus

DataFed Use-cases

- Integration with data ingestion pipelines (e.g. - instruments)
- User facility administration -> projects w/- allocations
- Data analytics
 - Rich metadata -> assembling labeled training datasets for ML / DL
- Standardization of domain-specific metadata via community defined schemas
- Provenance capture (parameters, etc.) in workflows -> traceability and reproducibility
- Smart research companion -> advise based on prior data

Development Roadmap

- High availability and reliability of core services
- Schema support for domain-specific metadata
- Data dissemination via publish / subscribe
- Bi-directional annotation
- Publishing data - DOI minting
- Data caching and replication
- Multimedia attachments (e.g. - thumbnails)
- Metrics - downloads, subscriptions, ratings, etc.

Summary

- DataFed - general purpose scientific data management system
- Federation of data repositories across facilities
- Aimed at:
 - Lowering data management burden
 - Improving scientific productivity and reproducibility
 - Facilitating cross-facility / -institutional data collaboration
 - Accelerating data-driven discovery
 - FAIR principle compliance
- Performant file transfers using Globus
- Simplified admin. & authn. (federated identity management)
- Designed with HPC and big data in mind

Acknowledgements

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Questions?

- Try it out:
 - <https://datafed.ornl.gov>
 - Requires Globus account
- Contact: stansberrydv@ornl.gov