

DataFed

A Federated Scientific Data Management System for Reproducible Science

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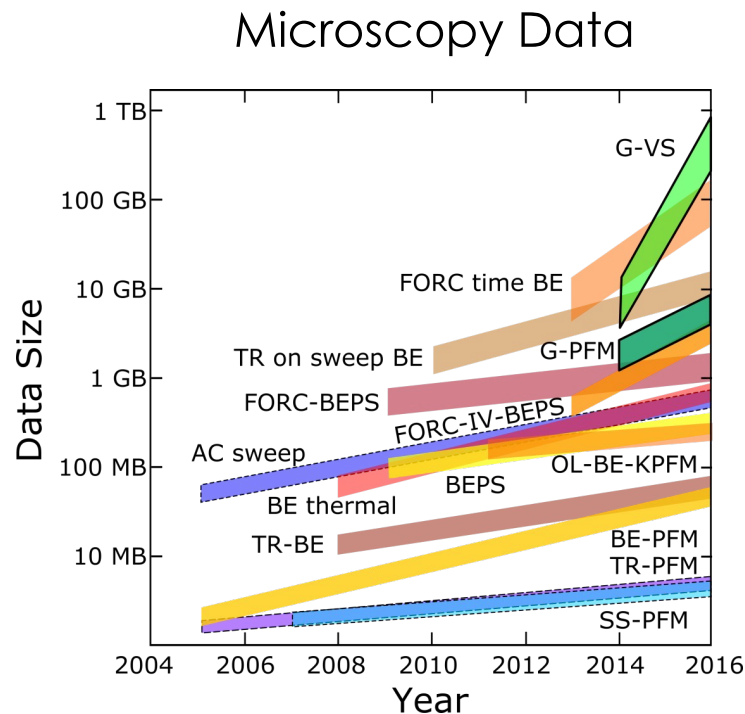
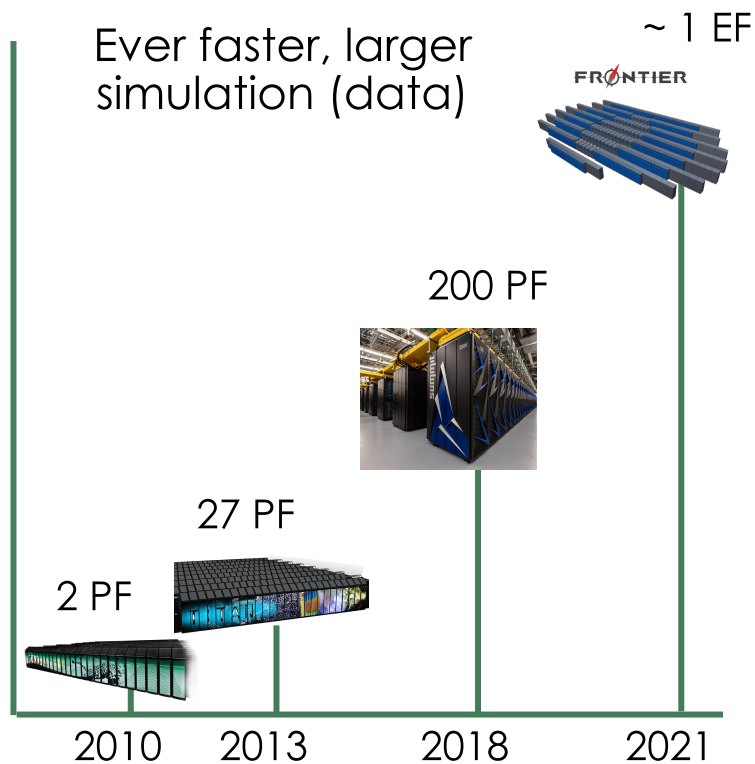
Advanced Data and Workflows Group
Oak Ridge Leadership Computing Facility

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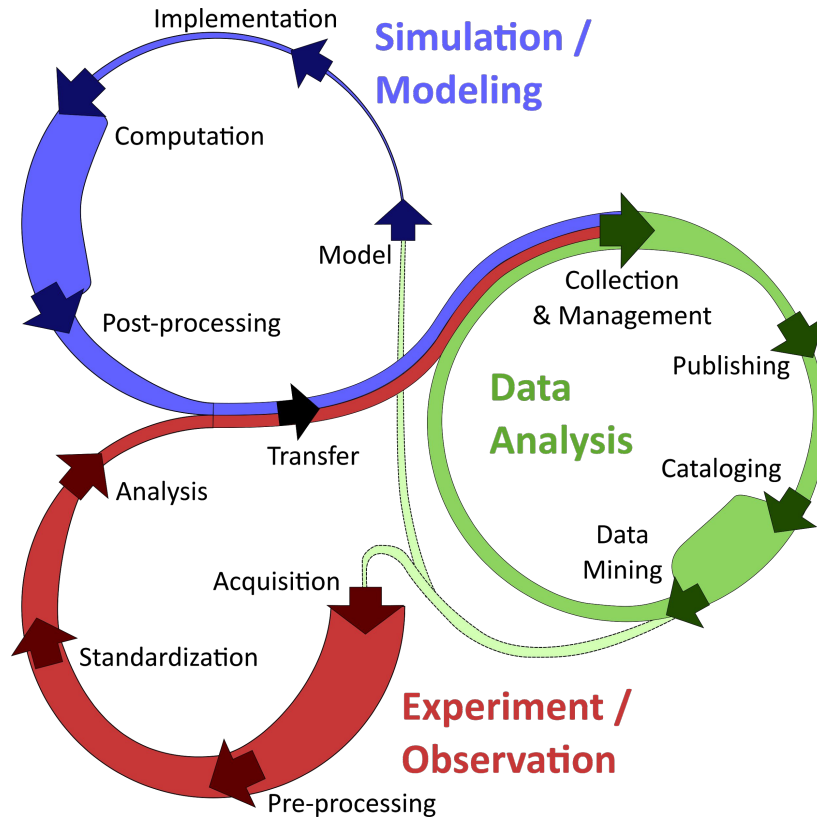
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Explosion in Data Volume, not (necessarily) Quality



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

Complex Data Lifecycle

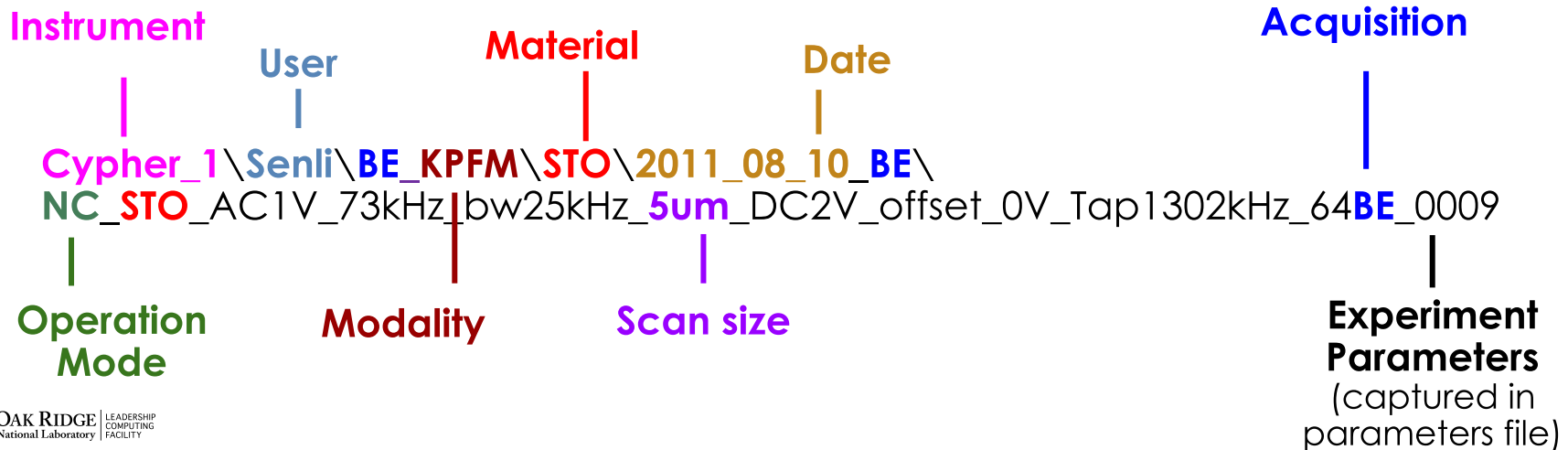


- Interplay of discovery paradigms
- Validation
- Reuse
- Global collaboration

Thickness
=
Data volume

Laborious Wrangling of Unstructured (Meta)data

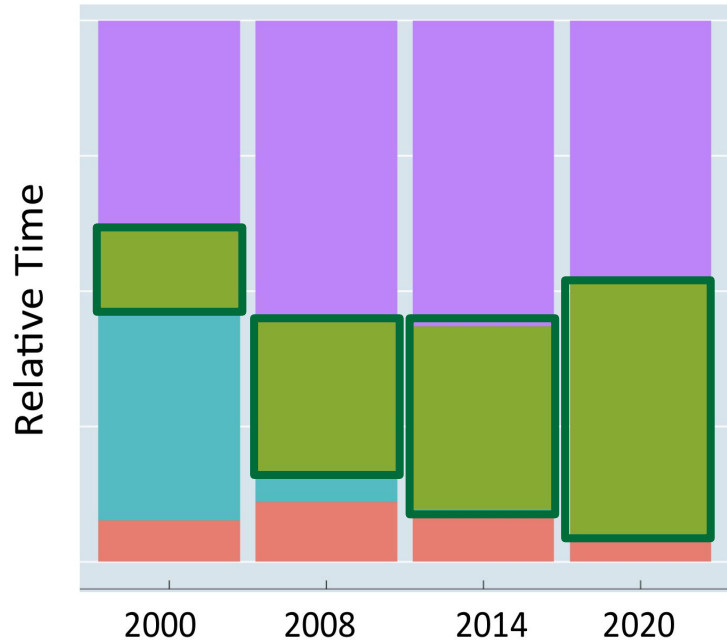
- Various and proprietary file formats
- Relevant metadata rarely available / indexed / searchable
 - Not all metadata may be available
 - Naming and structure varies by user and time
 - Most often embedded in file names



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

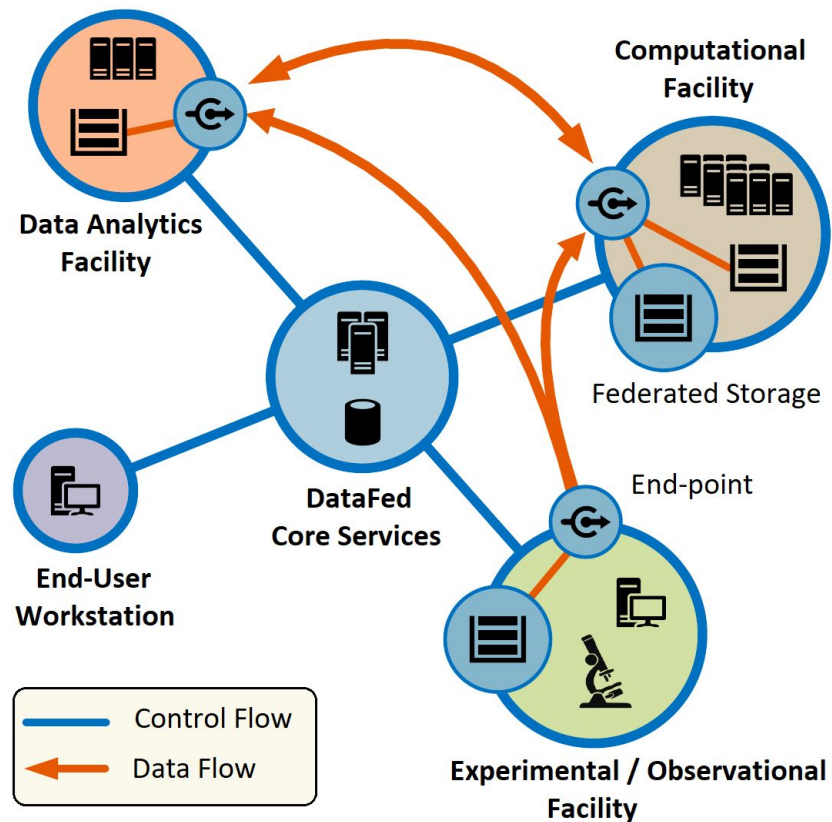
- Data handling application
- Unique identifiers for each record, collection, user, etc.
- Abstracts file system complexities (directories, paths, files,)
- Indexes metadata
 - General - author, creation date, size, provenance, etc.
 - Domain-specific
- Powerful searches
- Collaboration via fine-grained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

Scientific Data Management Systems Today

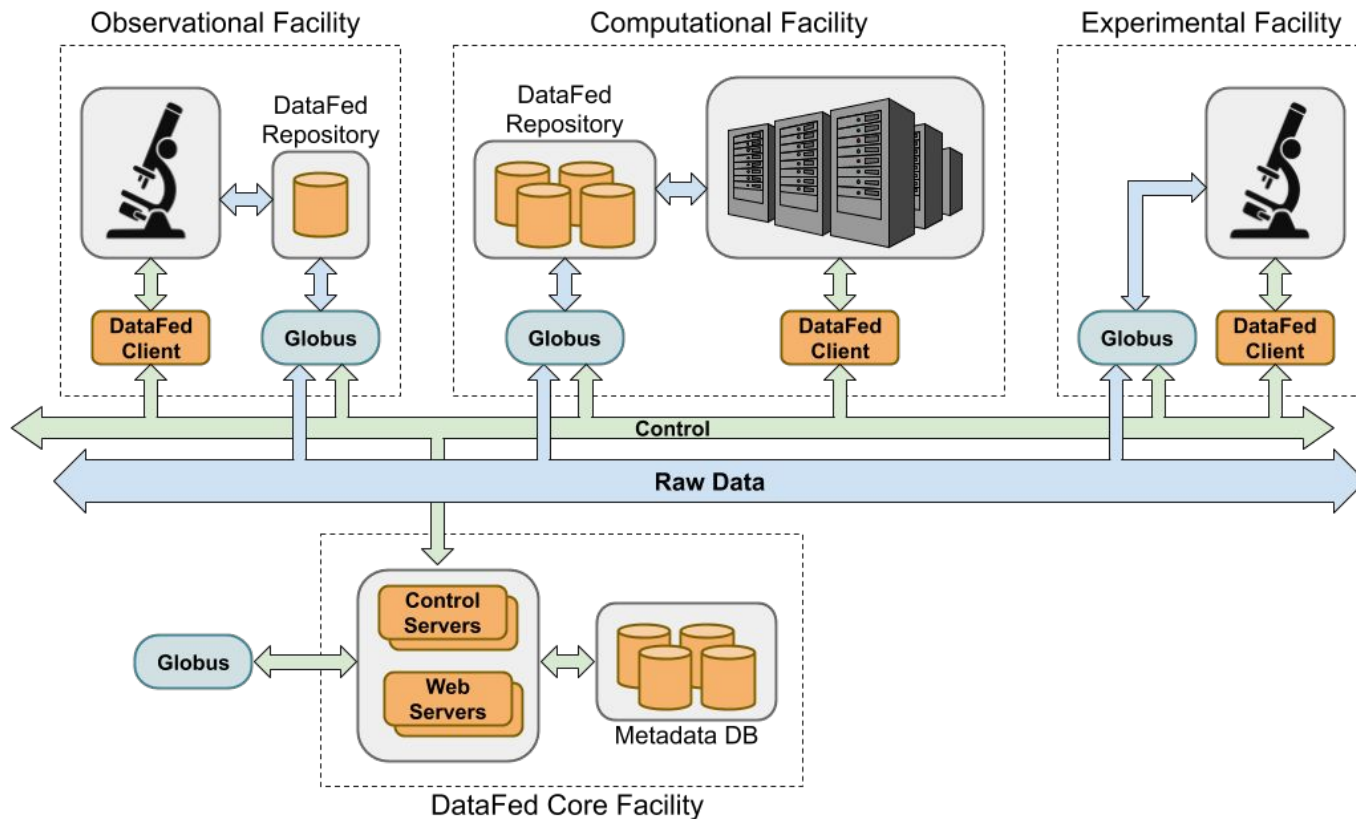
- Regularly used in commercial / production-oriented workflows
 - Highly specific to company / application
- Some used in academia
 - Rucio, iRODS, Clowder, Omero, K-Base, ...
 - Often rigid / tailored to specific scientific domains
 - Often using non-performant / non-scalable:
 - Data transfer - SCP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

DataFed

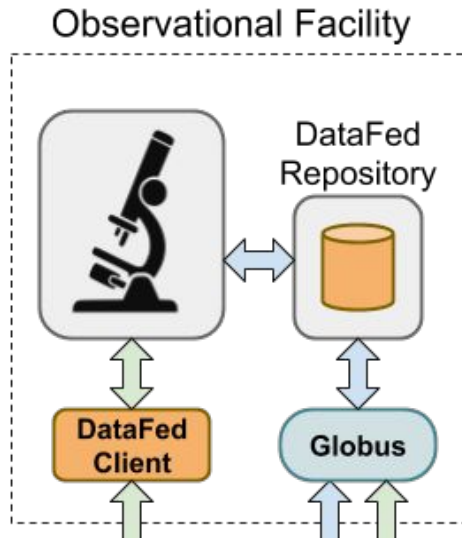
- General purpose, opt-in SDMS
- Federation of data repositories
- Using Globus for:
 - File transfers
 - Federated identity management
- Supports Findable, Accessible, Interoperable, Reusable (FAIR) principles
- Designed with HPC and big data in mind
- Spans facilities and organizations



DataFed - Federation of Data Repositories

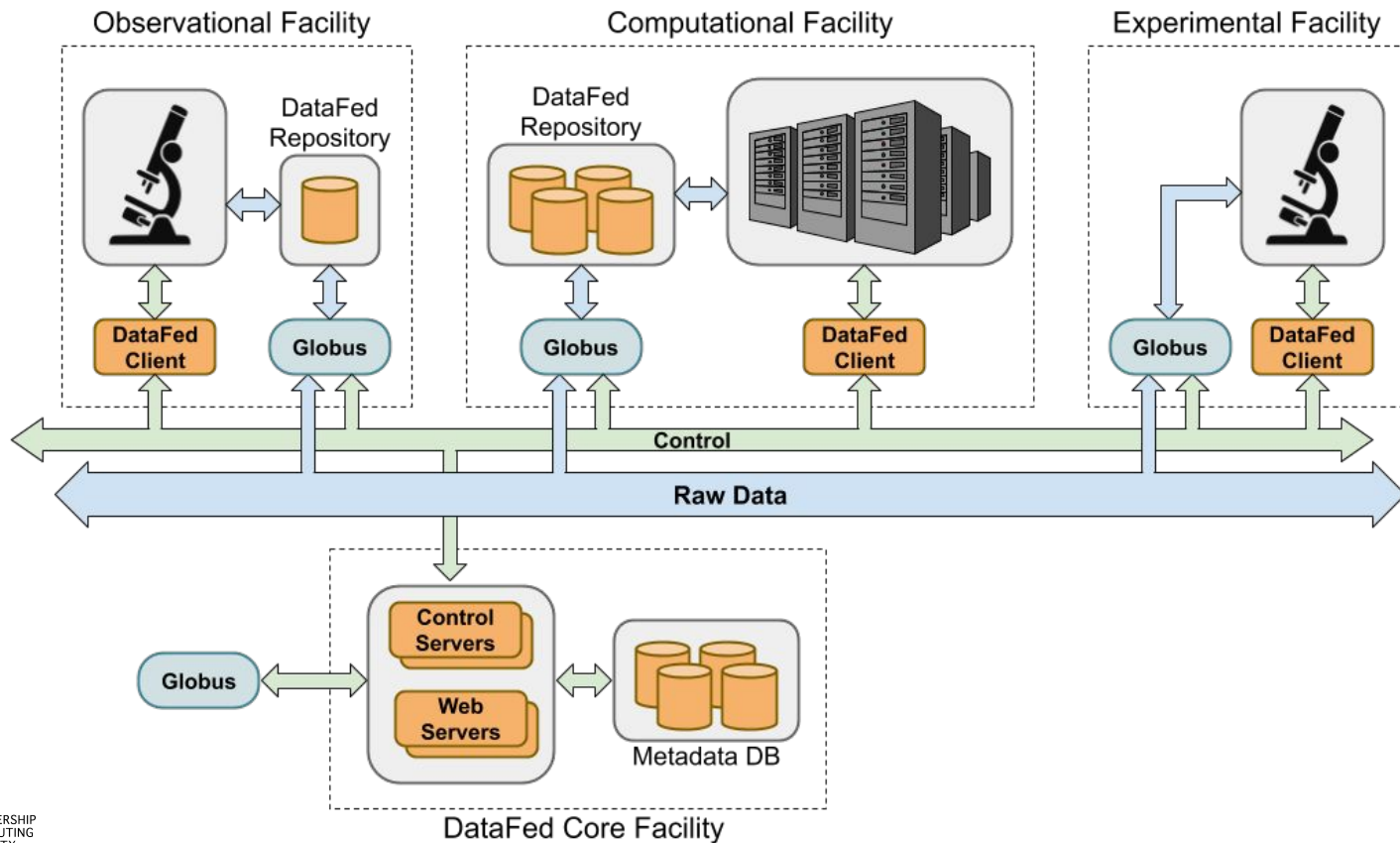


DataFed Repositories

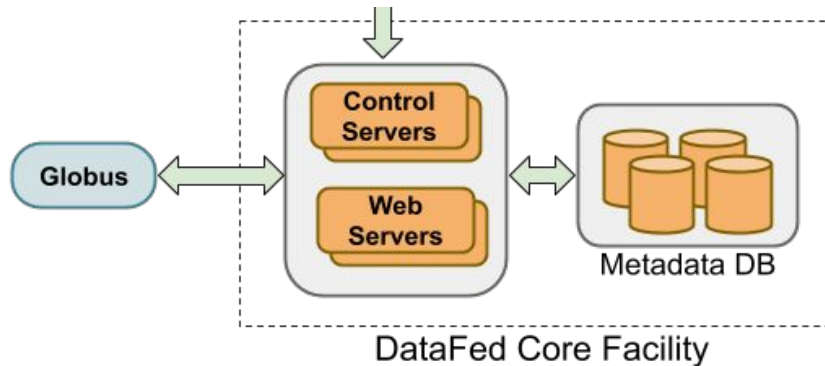


- Connect facility-local data storage to DataFed network via dedicated Globus endpoint
- Any file-system supported by Globus
- DataFed handles authorization, concurrency control, access control, etc.
- Raw binary data stays in repository
 - Managed by DataFed
 - Metadata in DataFed Database servers

DataFed - Federation of Data Repositories

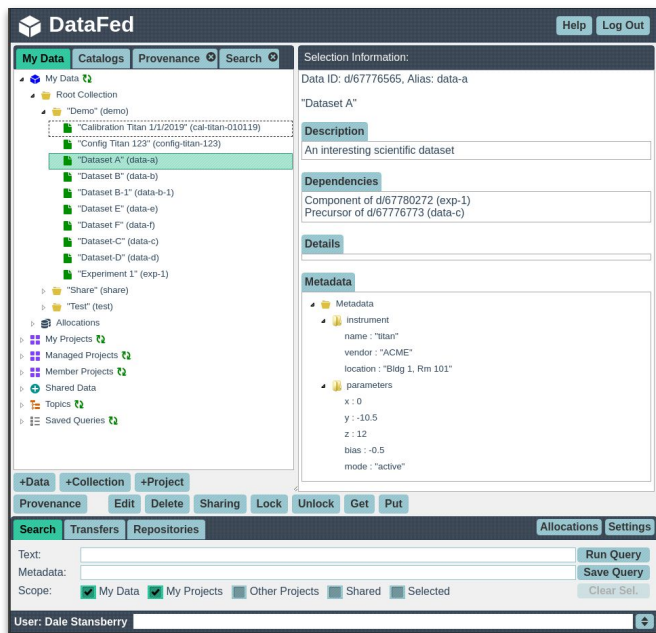


Core Services



- 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



Modern web application

```
3ub ~ 3ub@or-condo-login01:~ -- bash -- 77x36
>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/67777678 (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$
```

Command-line & Python package

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

General Metadata

The screenshot displays the DataFed v-0.7.2 web interface. The top navigation bar includes 'My Data', 'Catalogs', and 'Search'. The main content area is split into two panes. The left pane shows a tree view of the 'Root Collection' with several files, including the selected file 'VS126No2_BELine_0002'. The right pane shows the 'Selection Information' for the selected file, including its ID, alias, and a list of keywords. Below the selection information are sections for 'Provenance' (showing no relationships) and 'Details' (showing file properties like size and source). A toolbar at the bottom of the right pane contains buttons for 'Provenance', 'Edit', 'Delete', 'Sharing', 'Lock', 'Unlock', 'Get', 'Put', and 'Relocate'. At the bottom of the interface, there is a search section with input fields for 'ID/Alias' and 'Text', a 'Run Query' button, and a 'Scope' section with checkboxes for 'My Data', 'My Projects', 'Other Projects', 'Shared', and 'Selected'. There are also 'Allocations' and 'Settings' buttons.

- 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 displays the DataFed V-0.7.2 interface. The main window is divided into several sections:

- My Data**: A tree view showing a "Root Collection" containing several files. The file `"VS126No2_BEline_0002" (vs126no2_beline_0002)` is selected and highlighted in green.
- Selection Information**: A panel showing the metadata for the selected file. The metadata is structured as follows:
 - `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`
 - `0`: "Pt"
- Provenance**: A row of buttons for `Edit`, `Delete`, `Sharing`, `Lock`, `Unlock`, `Get`, `Put`, and `Relocate`.
- Search**: A section with input fields for `ID/Alias` and `Text`, and a `Metadata: *` field.
- Transfers**: A section with a `Scope` filter showing checkboxes for `My Data` (checked), `My Projects` (checked), `Other Projects`, `Shared`, and `Selected`.

Search

DataFed V-0.7.20 Help Log Out

My Data **Catalogs** **Search** ✕

- "PZT_cap_line_2um_0004" (pzt_cap_line_2um_0004)
- "PZTcer0005_BEline_0001" (pztcer0005_beline_0001)
- "PE60_spot2_5um_1Vac_pm20V..." (pe60_spot2_5um_1vac_pm20V...)
- "F186_BEline_0001" (f186_beline_0001)
- "29052016PZTFT4_BE_0002" (29052016pztft4_be_0002)
- "LSATLSMOPZTP1505LAOLSMOP..." (lsatlsmpztp1505laolsmpztp...)
- "6October2014PZT3000nm_0004" (6october2014pzt3000nm_0004)
- "JA0020_BElineV_after_0001" (ja0020_belinev_after_0001)
- "V181_BEline_0002" (v181_beline_0002)
- "PZT150J0012_BEline_0001" (pzt150j0012_beline_0001)
- "LSATLSMOPZTPLSATLSMOPZTP..." (lsatlsmpztp1505laolsmpztp...)
- "ITOPZTPN2800mTvergood_P..." (itopztpn2800mTvergood_P...)

Selection Information **Metadata**

- time_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

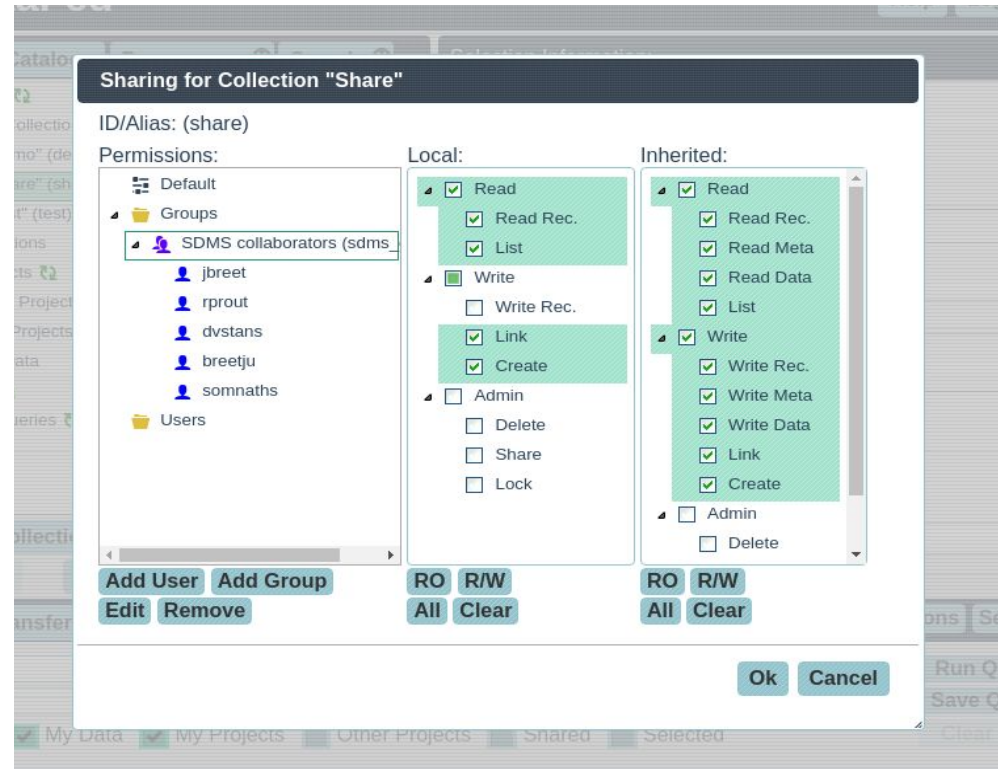
ID/Alias: Text: Run Query

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”
 - ...

The screenshot displays the DataFed Provenance interface. The main area shows a directed graph of data relationships. At the top, two nodes labeled 'cal-titan-010119' and 'config-titan-123' have arrows pointing to a central green node 'exp-1'. From 'exp-1', arrows point to 'data-b' and 'data-a'. 'data-b' has a red arrow pointing to 'data-b-1'. 'data-a' has a blue arrow pointing to 'data-c'. 'data-b-1' has a blue arrow pointing to 'data-e'. 'data-c' has a blue arrow pointing to 'data-d'. 'data-e' has a blue arrow pointing to 'data-f'. 'data-d' has a blue arrow pointing to 'data-f'. The 'data-a' node is highlighted with a blue circle. The right-hand panel contains the following information:

Selection Information:
Data ID: d/67776565, Alias: data-a
"Dataset A"

Description
An interesting scientific dataset

Dependencies
Component of d/67780272 (exp-1)
Precursor of d/67776773 (data-c)

Details
Keywords: data science, machine learning
Topic: N/A
Public Access: Disabled
Locked: No
Data Repo: core
Data Size: 0
Created: 4/3/19, 16:28
Updated: 4/3/19, 16:42
Owner: stansberrydv

Metadata
└─ Metadata
 └─ instrument
 name : "titan"
 vendor : "ACME"
 location : "Bldg 1, Rm 101"
 └─ parameters
 x : 0

Projects

New Project

ID:

Title:

Description:

Owner:

Sub-allocation:

Alloc. Size:

Members:

- breetju
- rprout
- shubhankar

Admins:

- somnaths

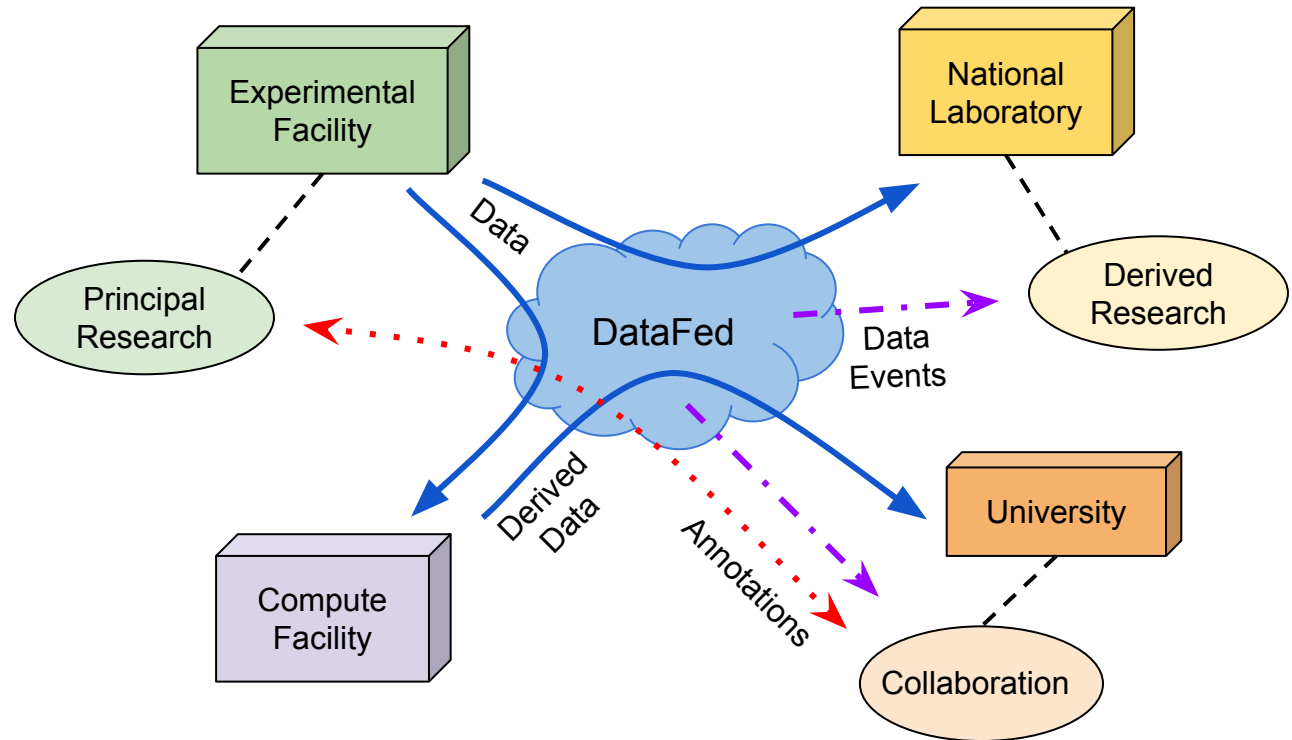
- Collective ownership of data
- Projects similar to user accounts
- Can be created by any user
- Assign admins and members
- Assign repository allocations
- Dedicated collection hierarchy
- Data owned by project
 - Member access based on admin defined permissions

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