A Systemic Approach to Facilitating Reproducibility via Federated, End-to-End Data Management

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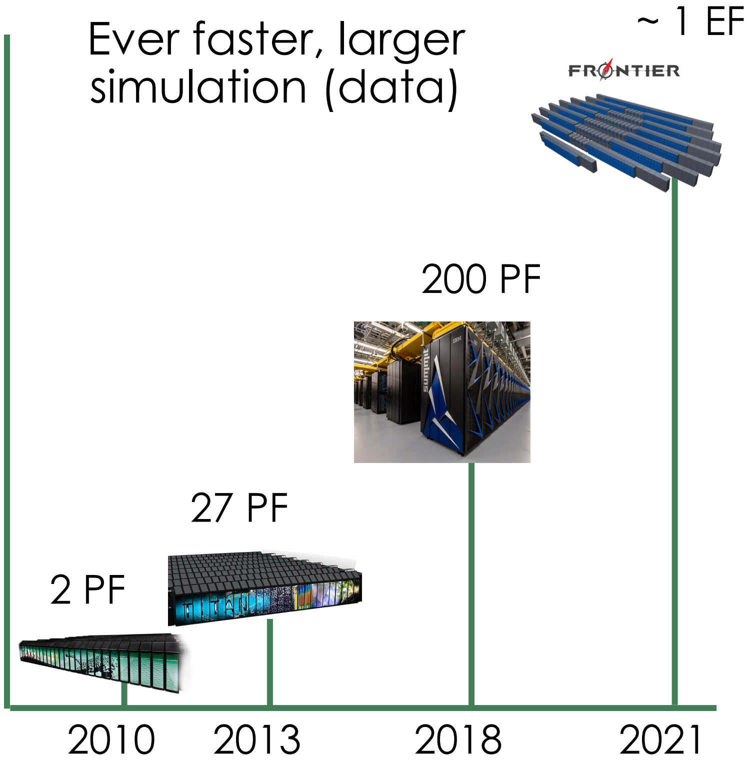
Explosion in Data Volume, not (necessarily) Quality



Ever faster, larger simulation (data)

2 PF

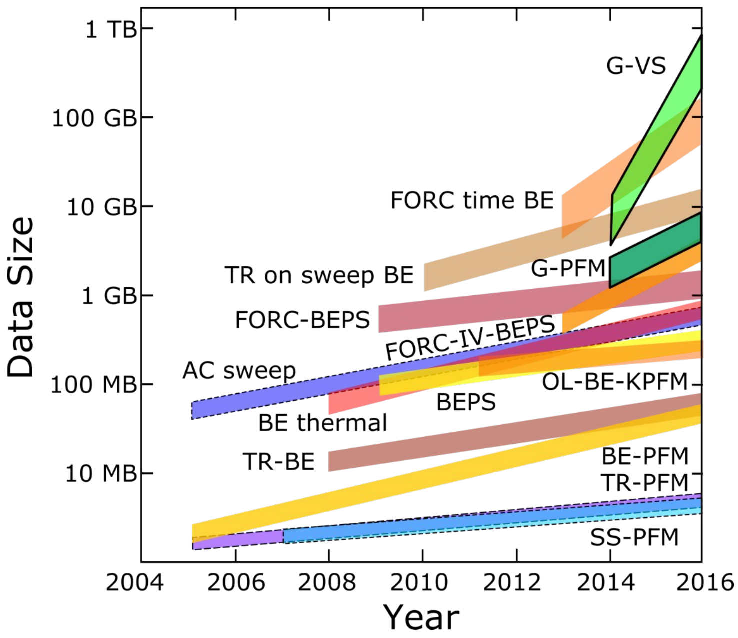
27 PF

200 PF

~ 1 EF

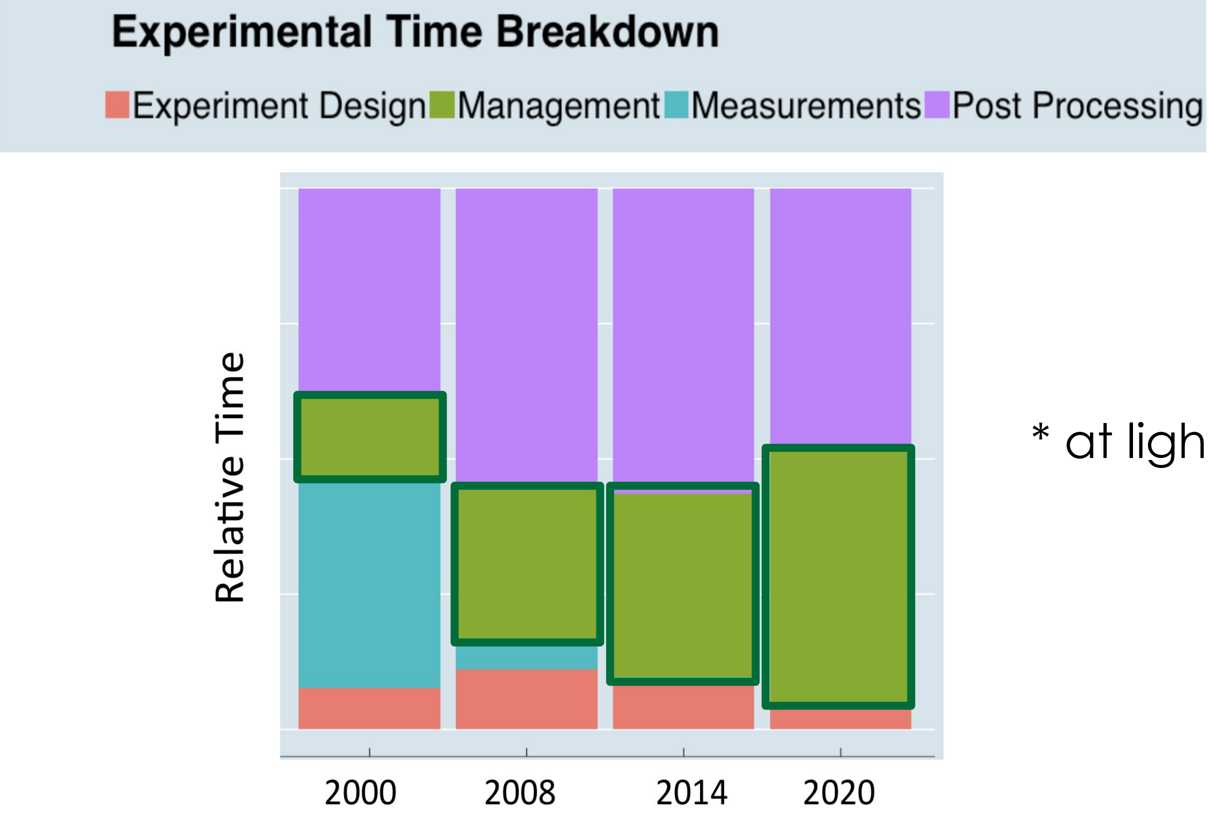
2010 2013 2018 2021

Microscopy Data



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

Explosion in Time Spent on Data Management



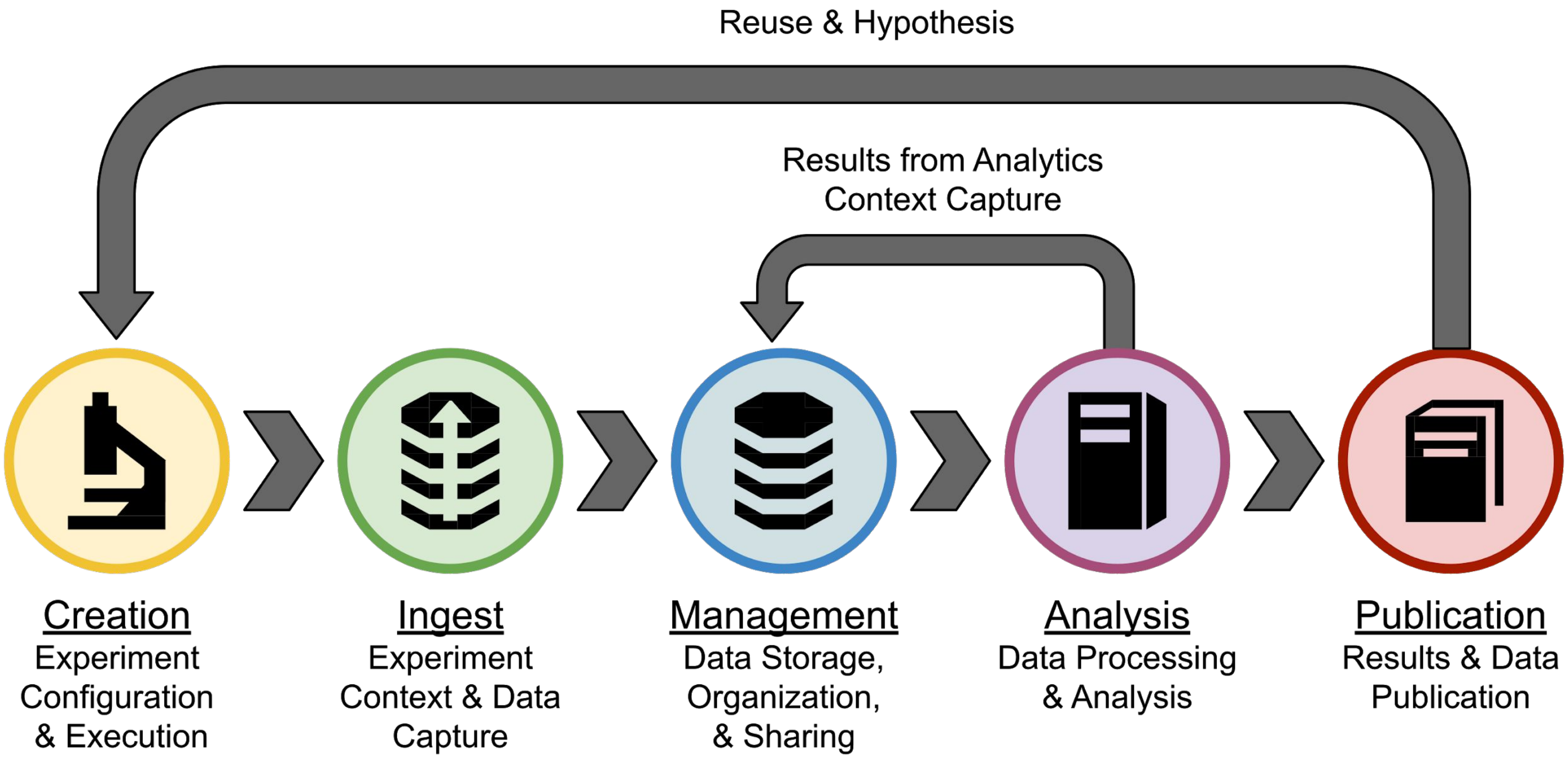
* at light sources

Figure from Kevin Mader
https://rawgit.com/4Quant/SRI2015/master/SRIPres.html#/

Lack of Data Infrastructure & ad-hoc Practices

- Metadata inadequately captured when generating data
  - Physical / electronic lab notebooks - rarely reconciled / findable
- Filesystem for data management
  - Metadata embedded into file paths
  - Sharing, searching, organization
- Thousands of data and metadata formats
- Emails, dropboxes, and portable storage for sharing data
- Dark data - majority of data never published / shared

Lifecycle of Scientific Datasets



Reuse & Hypothesis

Results from Analytics Context Capture

Creation
Experiment Configuration & Execution

Ingest
Experiment Context & Data Capture

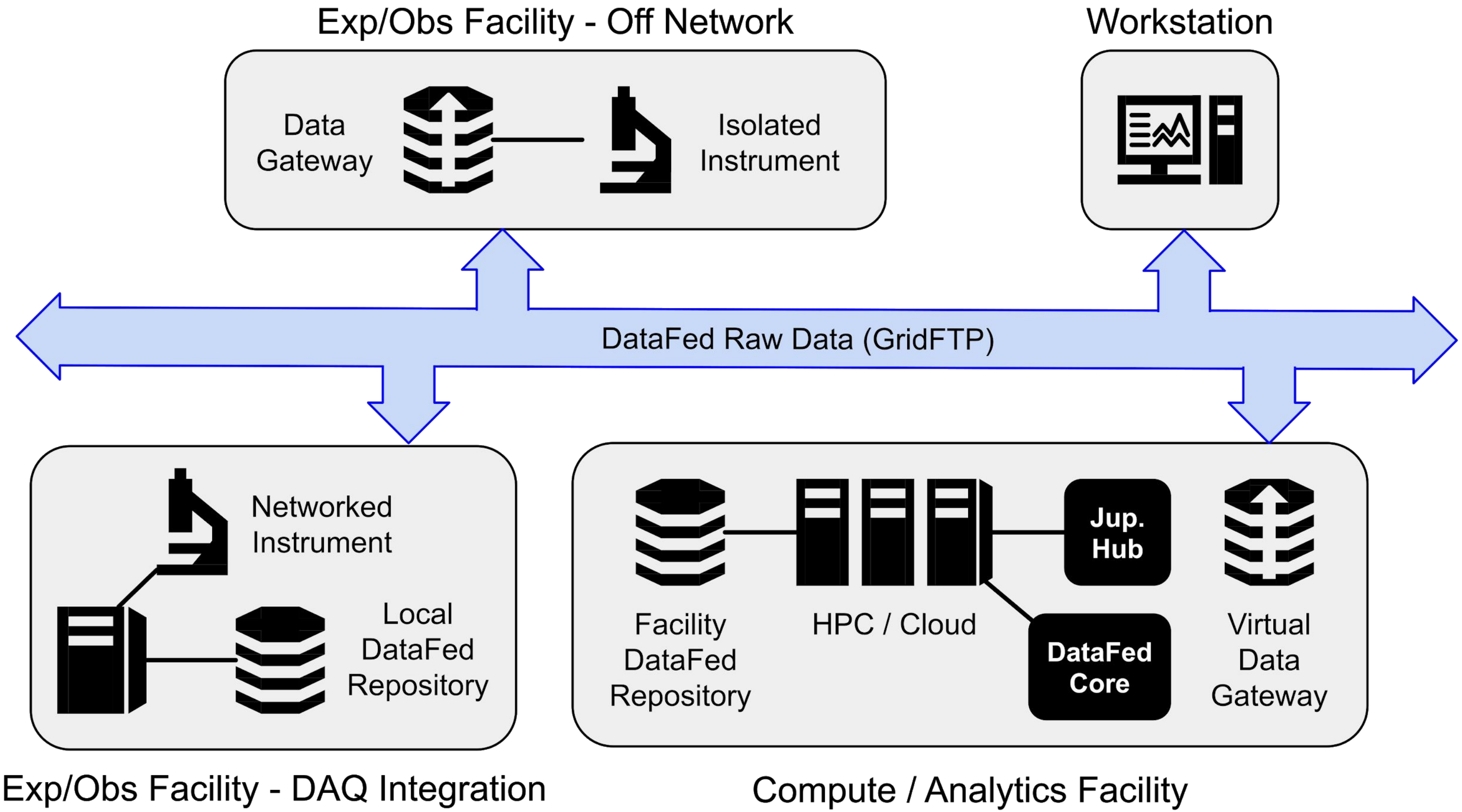
Management
Data Storage, Organization, & Sharing

Analysis
Data Processing & Analysis

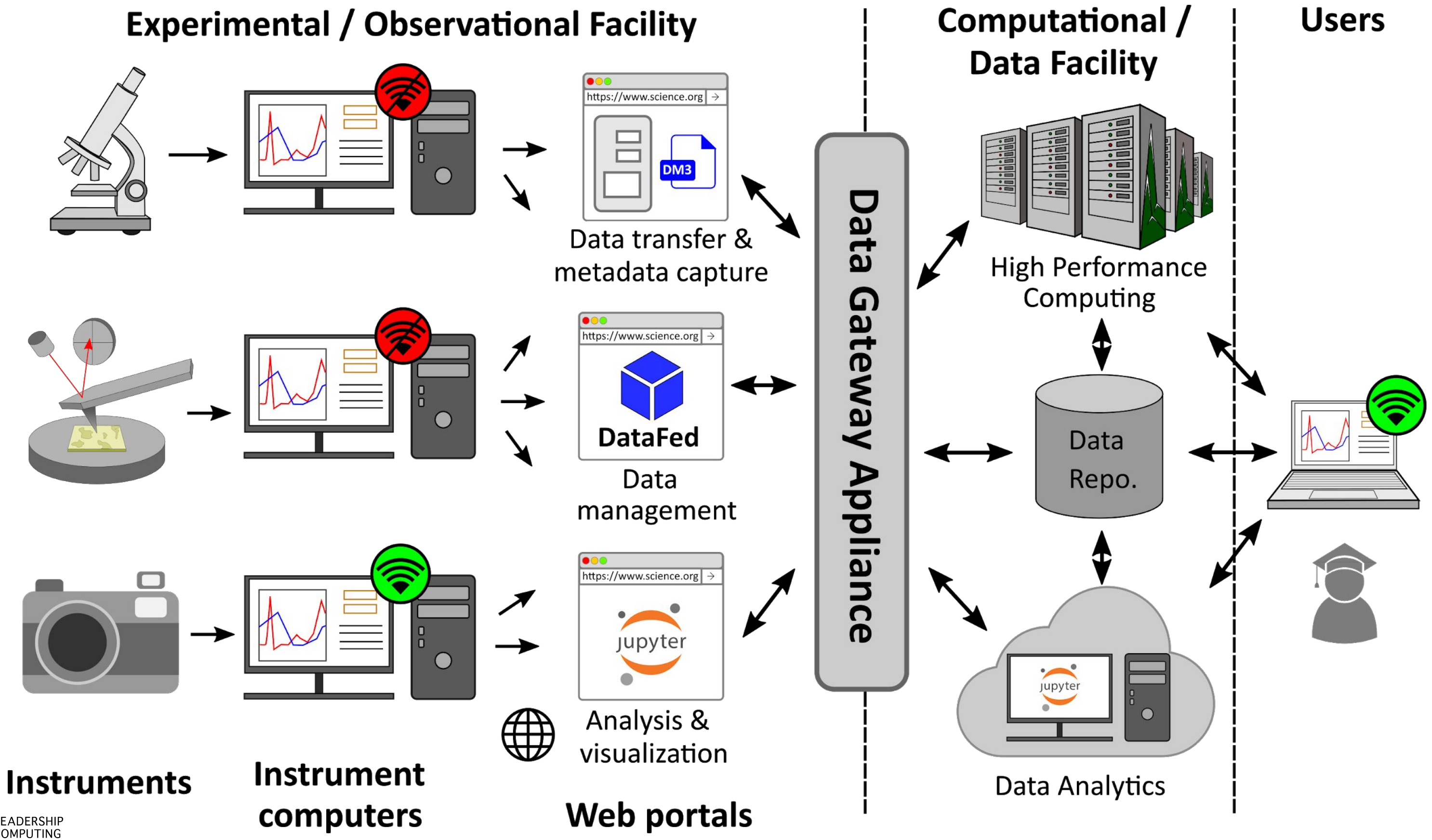
Publication
Results & Data Publication

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

Systemic Approach to Data Management


Exp/Obs Facility - Off Network
Data Gateway
Isolated Instrument
Workstation
DataFed Raw Data (GridFTP)
Networked Instrument
Local DataFed Repository
Exp/Obs Facility - DAQ Integration
Facility DataFed Repository
HPC / Cloud
Jup. Hub
DataFed Core
Virtual Data Gateway
Compute / Analytics Facility

Data Gateway - Data Ingest Tool



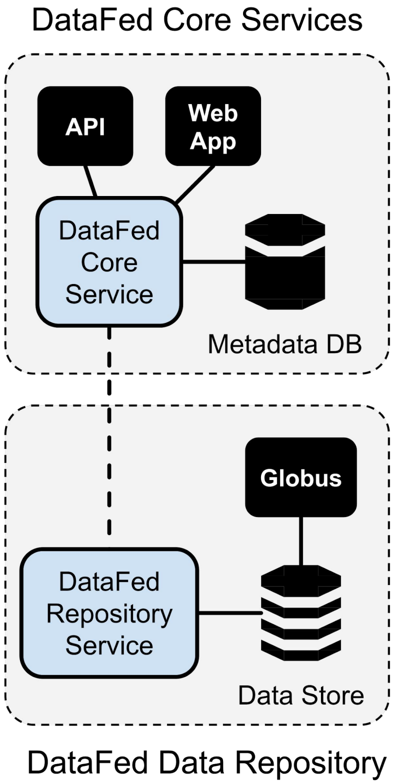
Data Gateway - Future Development

- Containers for data pre-processing
    - Extracting metadata, translating from proprietary formats, etc.
    - Isolates science code from Gateway
    - Repository of vetted codes / containers
- Virtual Gateway - Centralized deployment for users outside facilities
- Exposed API for automated ingest of data - long experiments
- Remote control / monitoring of instruments
- Trigger compute jobs for data processing on HPC

DataFed - Scientific Data Management System

- 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
- Fine-grained access control
- Globus for:
  - Data movement (Grid-FTP)
  - Authentication (federated identity management)

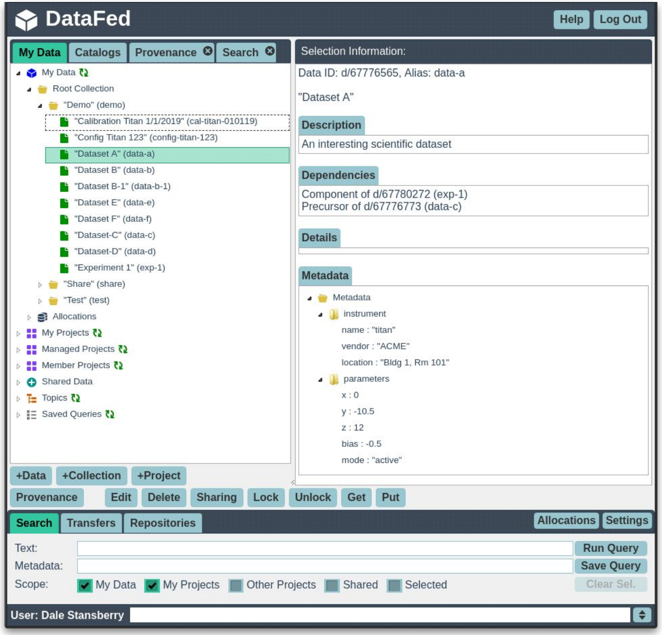
DataFed Core Services and Example Repository



- DataFed Core Services:
  - Control servers
  - Web servers
  - Database
  - DataFed handles authorization, concurrency control, access control, etc.

- Example DataFed Data Repository:
  - Any file-system supported by Globus
  - Raw binary data stays in repository
  - Metadata only in DataFed Database

DataFed Interface - Web Portal and CLI



My Data
Root Collection
"Demo" (demo)
"Calibration Titan 1/1/2019" (cal-titan-010119)
"Config Titan 123" (config-titan-123)
"Dataset A" (data-a)
"Dataset B" (data-b)
"Dataset B-1" (data-b-1)
"Dataset E" (data-e)
"Dataset F" (data-f)
"Dataset-C" (data-c)
"Dataset-D" (data-d)
"Experiment 1" (exp-1)
"Share" (share)
"Test" (test)
Allocations
My Projects
Managed Projects
Member Projects
Shared Data
Topics
Saved Queries

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

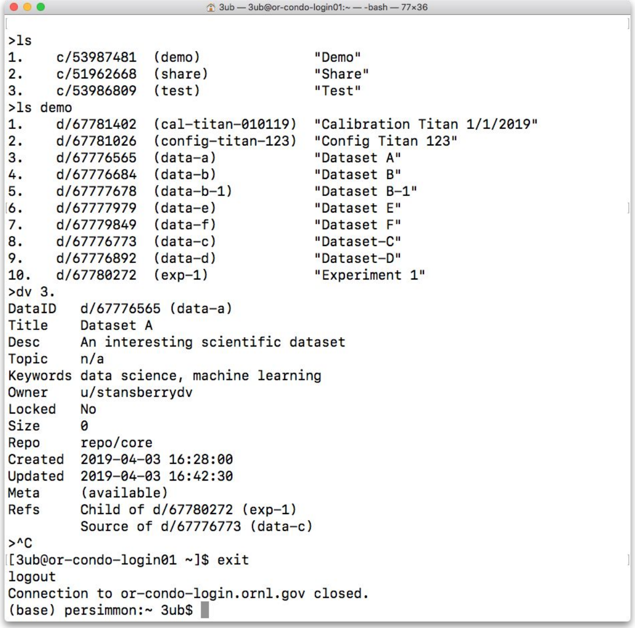
Metadata

Metadata
instrument
name : "titan"
vendor : "ACME"
location : "Bldg 1, Rm 101"
parameters
x : 0
y : -10.5
z : 12
bias : -0.5
mode : "active"

Text:
Metadata:
Scope: ☑ My Data ☑ My Projects □ Other Projects □ Shared □ Selected

User: Dale Stansberry

Modern web application



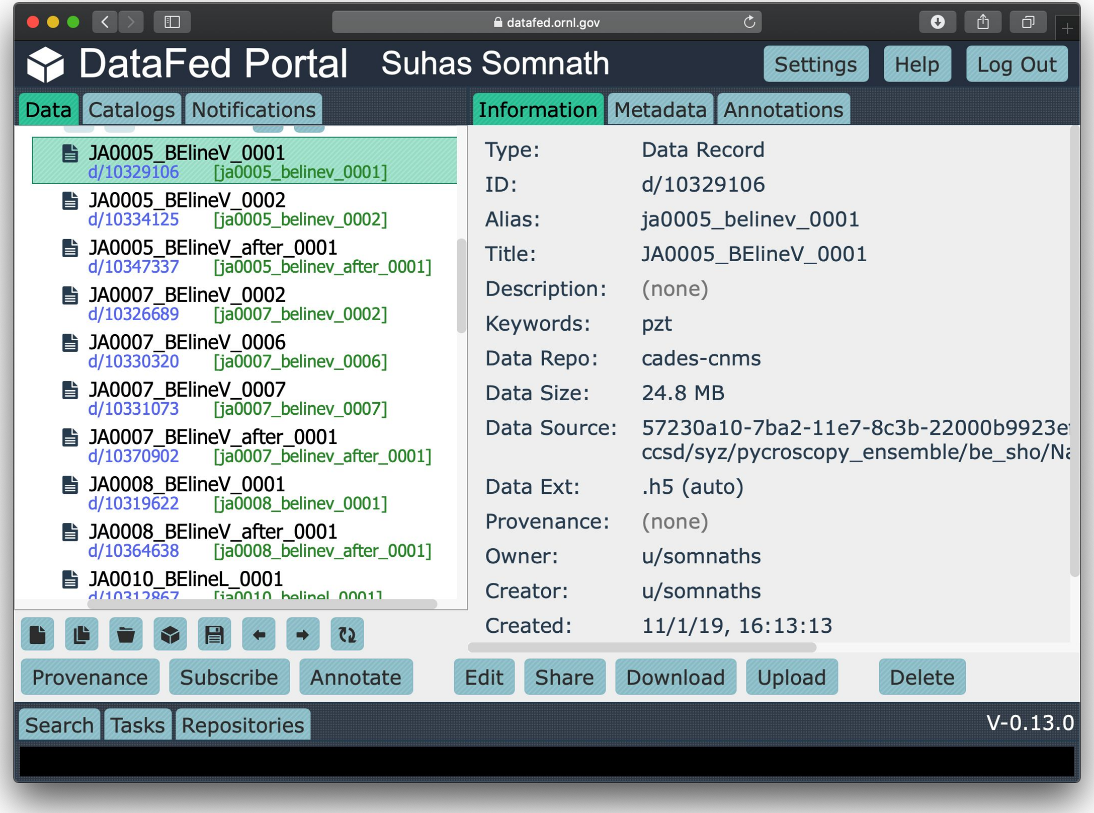
3ub — 3ub@or-condo-login01:~ — -bash — 77×36

```
>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



JA0005_BElineV_0001
d/10329106 [ja0005_belinev_0001]

JA0005_BElineV_0002
d/10334125 [ja0005_belinev_0002]

JA0005_BElineV_after_0001
d/10347337 [ja0005_belinev_after_0001]

JA0007_BElineV_0002
d/10326689 [ja0007_belinev_0002]

JA0007_BElineV_0006
d/10330320 [ja0007_belinev_0006]

JA0007_BElineV_0007
d/10331073 [ja0007_belinev_0007]

JA0007_BElineV_after_0001
d/10370902 [ja0007_belinev_after_0001]

JA0008_BElineV_0001
d/10319622 [ja0008_belinev_0001]

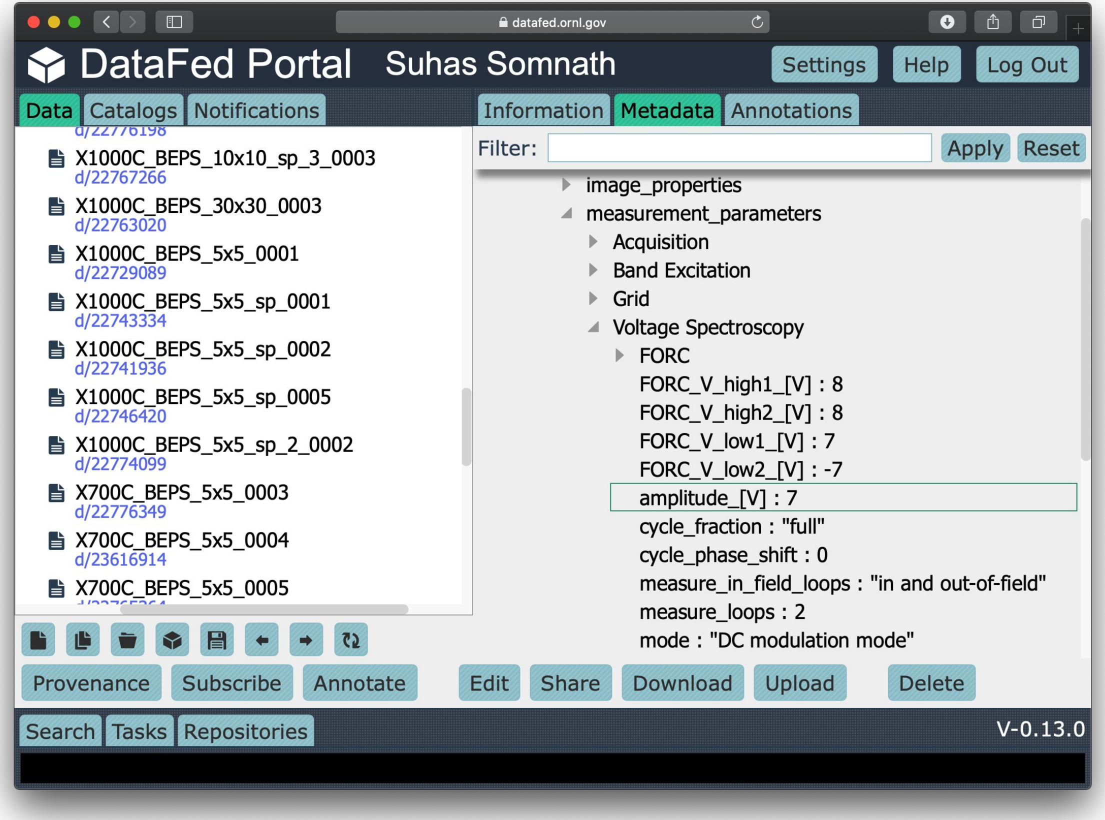
JA0008_BElineV_after_0001
d/10364638 [ja0008_belinev_after_0001]

JA0010_BElineL_0001
d/10312867 [ja0010_belinel_0001]

Type:	Data Record
ID:	d/10329106
Alias:	ja0005_belinev_0001
Title:	JA0005_BElineV_0001
Description:	(none)
Keywords:	pzt
Data Repo:	cades-cnms
Data Size:	24.8 MB
Data Source:	57230a10-7ba2-11e7-8c3b-22000b9923e ccsd/syz/pycroscopy_ensemble/be_sho/Na
Data Ext:	.h5 (auto)
Provenance:	(none)
Owner:	u/somnaths
Creator:	u/somnaths
Created:	11/1/19, 16:13:13

- Owner
- Repository
- Size
- Date / time
- Keywords
- Tags
- Title
- Description
- more…
- Searchable

Domain-specific Metadata

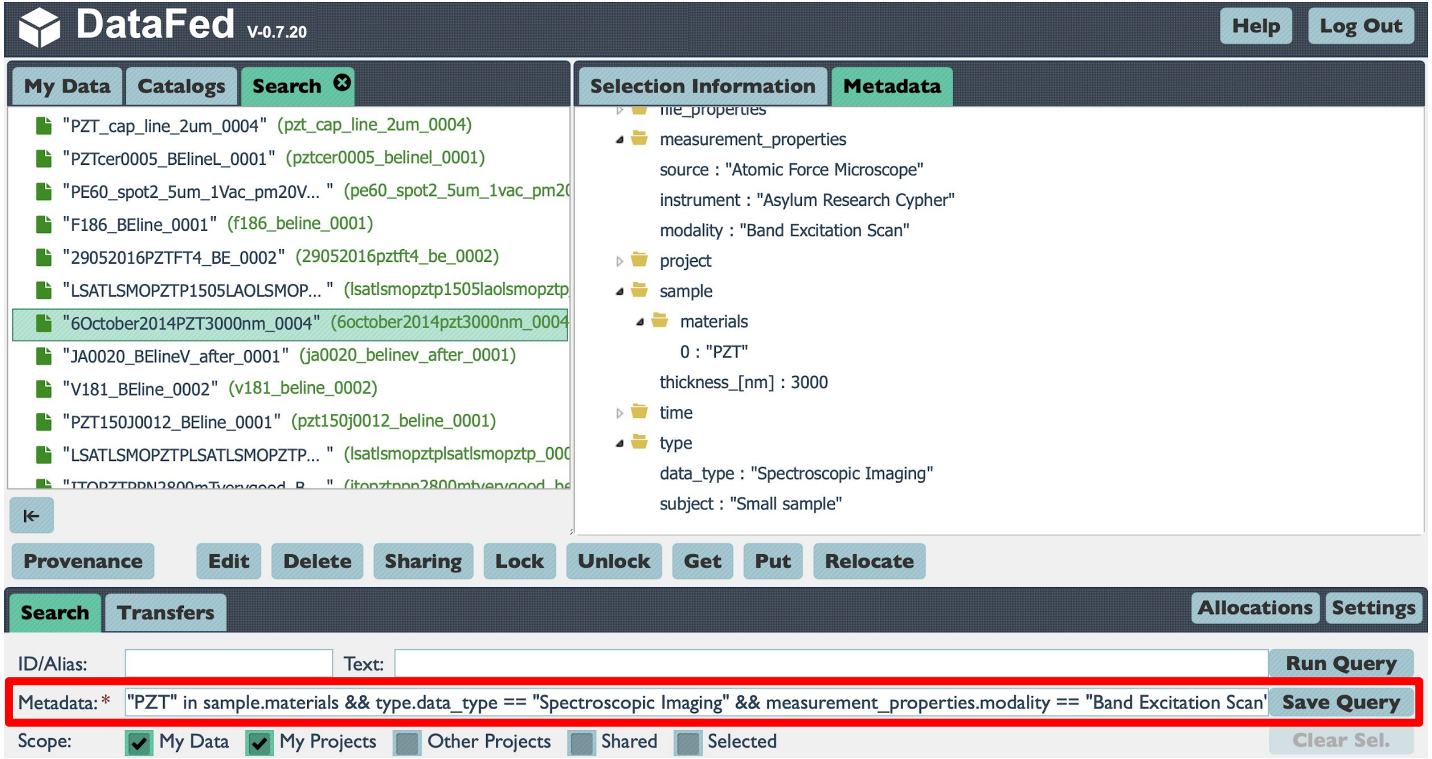


d/22776198
X1000C_BEPS_10x10_sp_3_0003
d/22767266
X1000C_BEPS_30x30_0003
d/22763020
X1000C_BEPS_5x5_0001
d/22729089
X1000C_BEPS_5x5_sp_0001
d/22743334
X1000C_BEPS_5x5_sp_0002
d/22741936
X1000C_BEPS_5x5_sp_0005
d/22746420
X1000C_BEPS_5x5_sp_2_0002
d/22774099
X700C_BEPS_5x5_0003
d/22776349
X700C_BEPS_5x5_0004
d/23616914
X700C_BEPS_5x5_0005

```
▸ image_properties
▾ measurement_parameters
    ▸ Acquisition
    ▸ Band Excitation
    ▸ Grid
    ▾ Voltage Spectroscopy
        ▸ FORC
          FORC_V_high1_[V] : 8
          FORC_V_high2_[V] : 8
          FORC_V_low1_[V] : 7
          FORC_V_low2_[V] : -7
          amplitude_[V] : 7
          cycle_fraction : "full"
          cycle_phase_shift : 0
          measure_in_field_loops : "in and out-of-field"
          measure_loops : 2
          mode : "DC modulation mode"
```

- Arbitrary tree
- String, numeric, array values
- Searchable
- Community defined schemas upcoming
- No need to embed metadata in file names

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_pm2(
"F186_BEline_0001" (f186_beline_0001)
"29052016PZTFT4_BE_0002" (29052016pztft4_be_0002)
"LSATLSMOPZTP1505LAOLSMOP... " (lsatlsmopztp1505laolsmopztp
"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... " (lsatlsmopztplsatlsmopztp_000
"ITOPZTPPN2800mTverygood_B... " (itopztppn2800mtverygood_be

```
▷ 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"
```

ID/Alias:

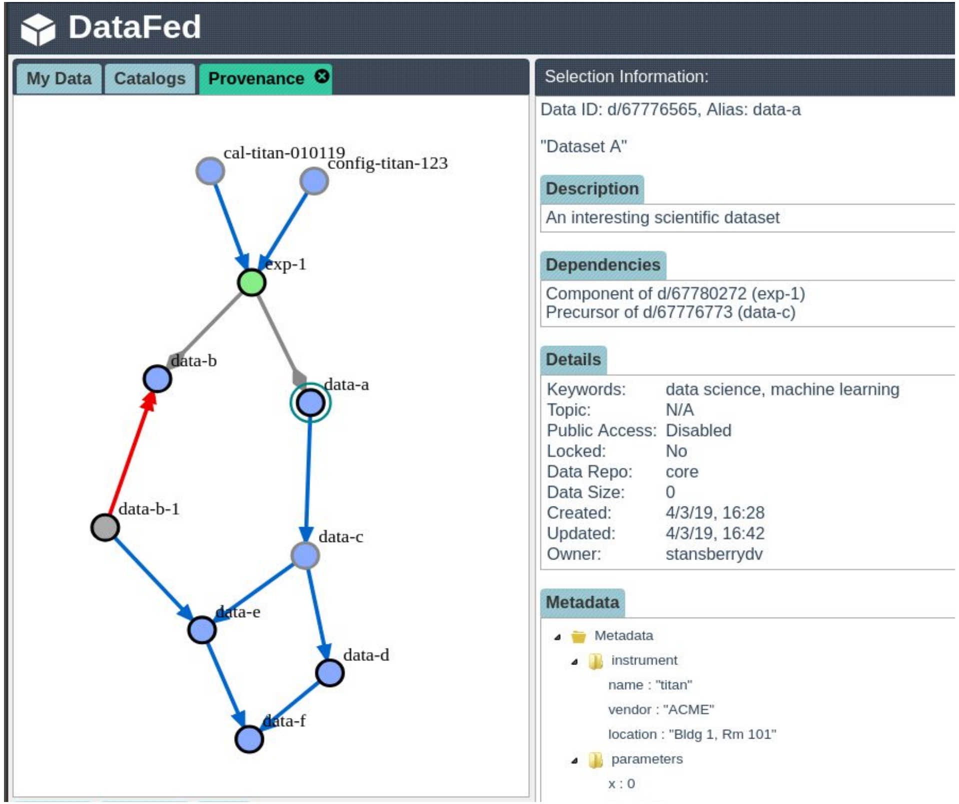
Text:

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

Scope: ☑ My Data ☑ My Projects □ Other Projects □ Shared □ Selected

Provenance Capture

- Currently supports:
  - "Derived from"
  - "Component of"
  - "New version of"
- More coming soon
- User-defined relationships
  - "Calibration associated with"
  - …



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Dependencies

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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

DataFed Applied to Simulations / Modelling

```
1 datafed data get input_parms_record ./parameters.txt
2 simulation run --input ./parameters.txt
3 context.json = parse(parameters)  AND/OR
3 context.json = extract_metadata(results_files)
4 datafed data create \
               --metadata context.json \
               --raw-data-file results_files.tar \
               “New_sim_results”
```

- Line 1 - Unambiguous identification of input files
- Line 4 - One line to create DataFed record, provide metadata, upload data
- Works for parameter sweeps - multiple similar simulation runs
- Towards reproducible simulation workflow
- Ease collection of training data for machine learning / deep learning

DataFed Applied to Artificial Intelligence

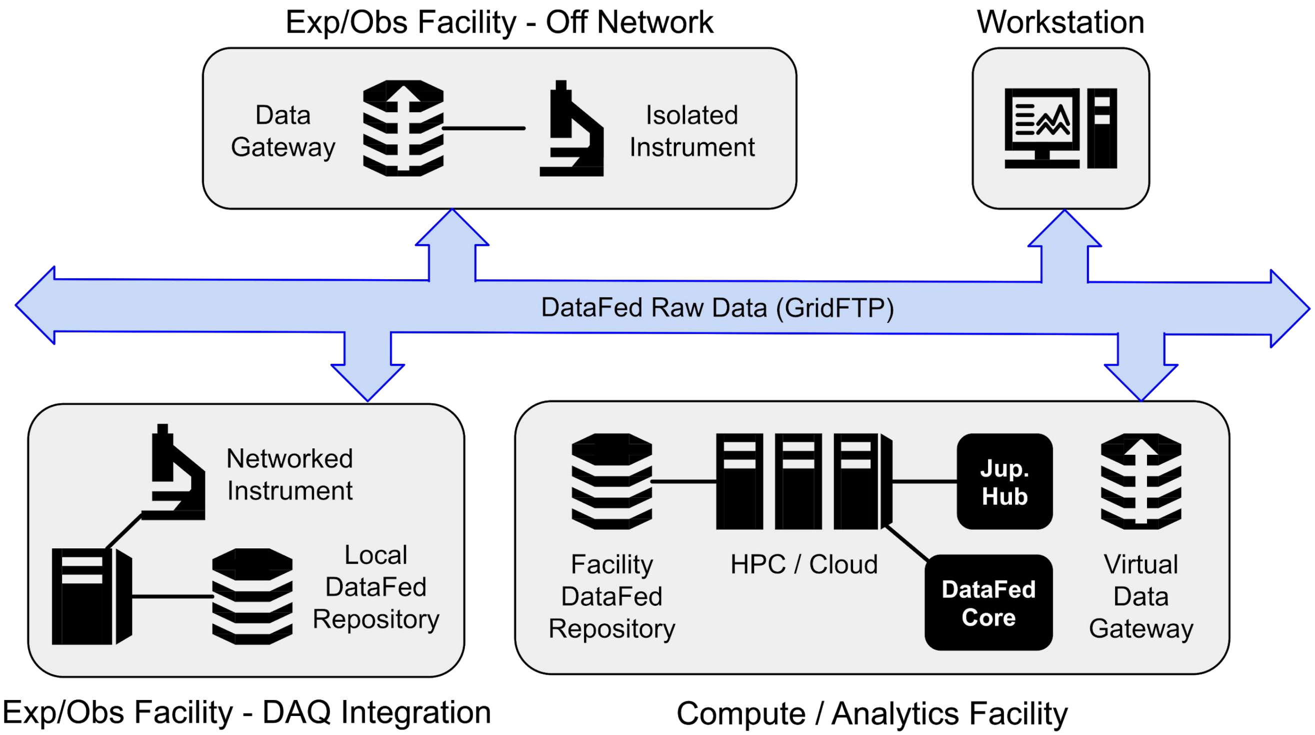
```
1 datafed data get training_coll ./train
2 datafed data get input_parms_record ./parameters.txt
3 python script.py --train ./train --parms ./parms.json
4 context.json = parse(output.log)
5 datafed data create \
                --metadata context.json \
                --raw-data-file results_files.tar \
                “New_sim_results”
```

- Line 1 - Collaborative collection of datasets
- Line 1 - Easily staging data located at multiple repositories at file-system
- Line 5 - One line to create DataFed record, provide metadata, upload data
- Assemble training datasets using tags and keywords of data records

Data Infrastructure Applied to Experimental Sciences

- Data Gateway servers facilitate (at instrument):
  - Data Ingest
    - Consistent capture of metadata / context wrt experiments
    - Drag-and-drop upload to data repository
    - Automated upload of data for long-running experiments
  - Data Management web portal piped in
  - Data Analytics web portal (JupyterHub) piped in
  - Automated data processing jobs on HPC
  - Instrument remote control
- DataFed - multi-user, -modal, -instrument data correlations

Summary



Exp/Obs Facility - Off Network
Data Gateway
Isolated Instrument
Workstation
DataFed Raw Data (GridFTP)
Networked Instrument
Local DataFed Repository
Exp/Obs Facility - DAQ Integration
Facility DataFed Repository
HPC / Cloud
Jup. Hub
DataFed Core
Virtual Data Gateway
Compute / Analytics Facility

DataFed:

- Data backplane
- Federation of repositories
- Rich metadata, provenance
- Data sharing, search, movement, staging, etc.

Data Gateway:

- Data upload
- Metadata capture
- Portal to data services

Acknowledgements

This research used resources of the Oak Ridge Leadership Computing Facility (OLCF) and of the Compute and Data Environment for Science (CADES) at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05- 00OR22725.

Questions?

- Try out DataFed:
  - https://datafed.ornl.gov
  - Requires Globus account
  - Contact: stansberrydv@ornl.gov
- somnaths@ornl.gov