Materials Data Facility:
A Distributed Model for the Materials Data Community

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materialsdatafacility.org
globus.org

Materials Genome Initiative

NIST National Institute of Standards and Technology U.S. Department of Commerce

CHiMaD Center for Hierarchical Materials Design

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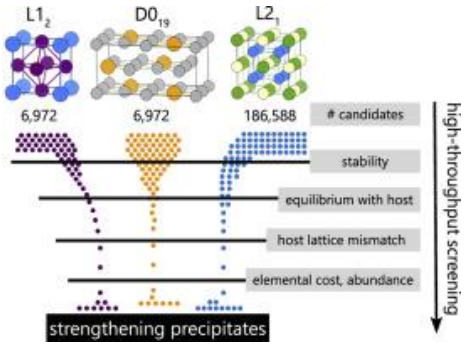
Argonne NATIONAL LABORATORY

Data-Intensive Materials Science

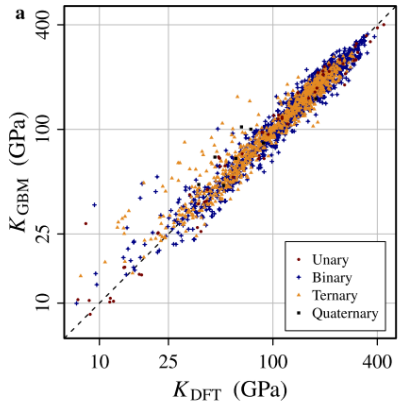
Materials Databases

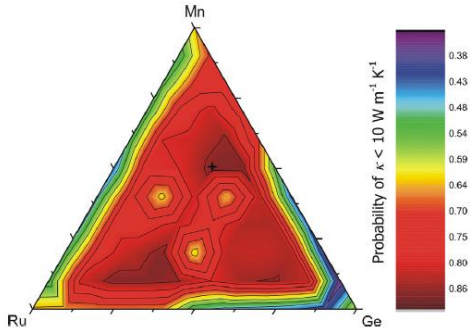
High-Throughput Screening



Kirklin *et al*. Acta Mat. (2016)

Machine Learning

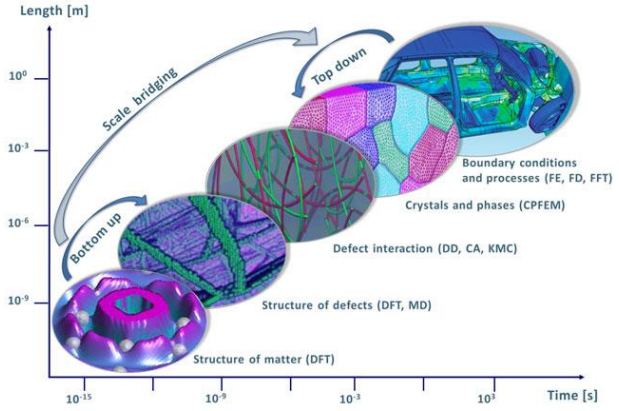




de Jong *et al*. Sci Rep. (2016)

Sparks *et al*. Scr. Mat. (2015)

Multi-scale Modeling



https://www.mpg.de/

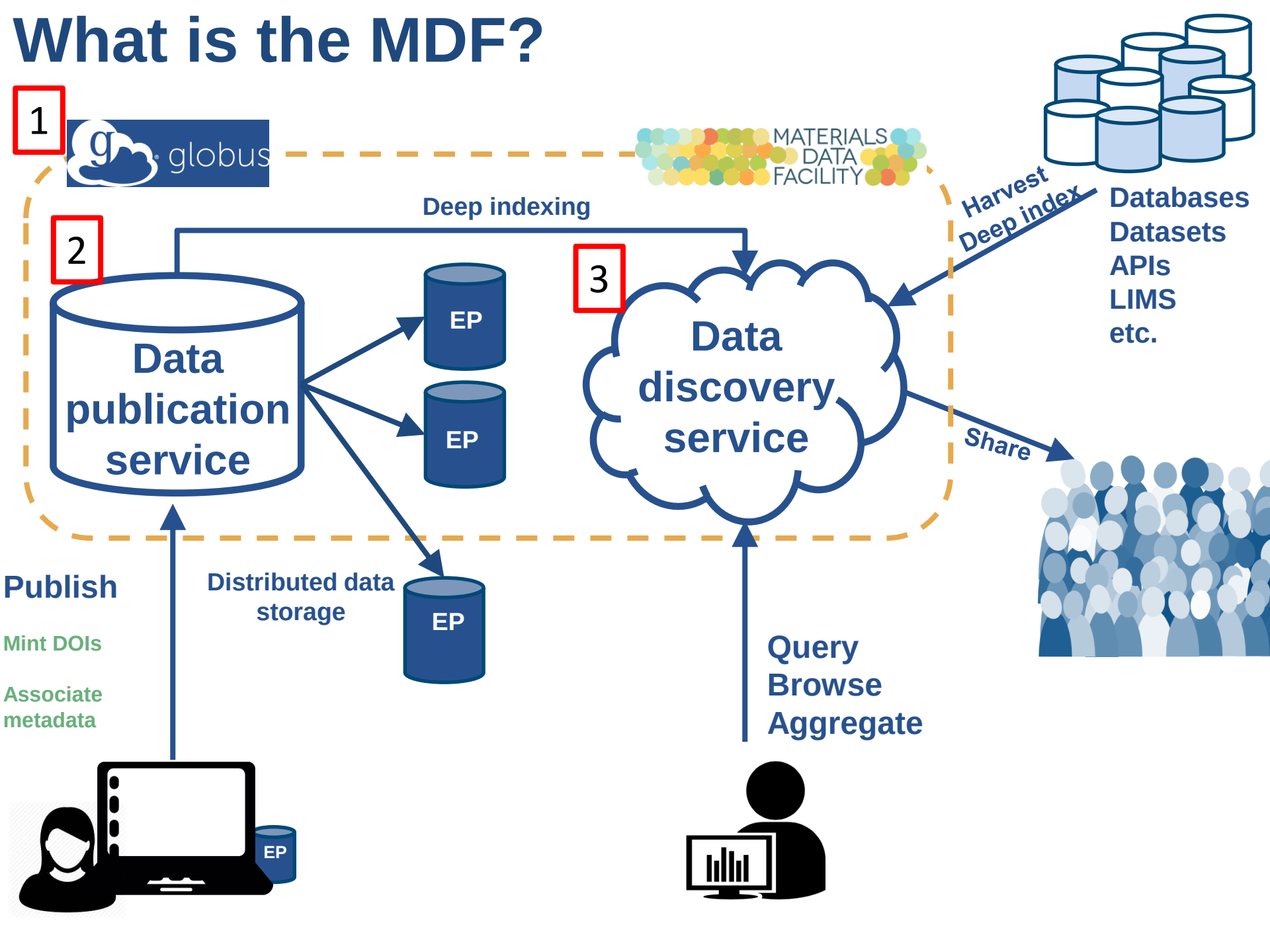
Data-Intensive Materials Science

Science is becoming limited by the ability to handle data

- Where to get it?
- How to selectively share it?
- Where to store it?
- How to know what it is?
- How to build software that uses it?
- How to get others to share theirs?
- How to keep track of provenance?
- ….?

Our goal is to create infrastructure that provides easy answers to these questions

What is the MDF?



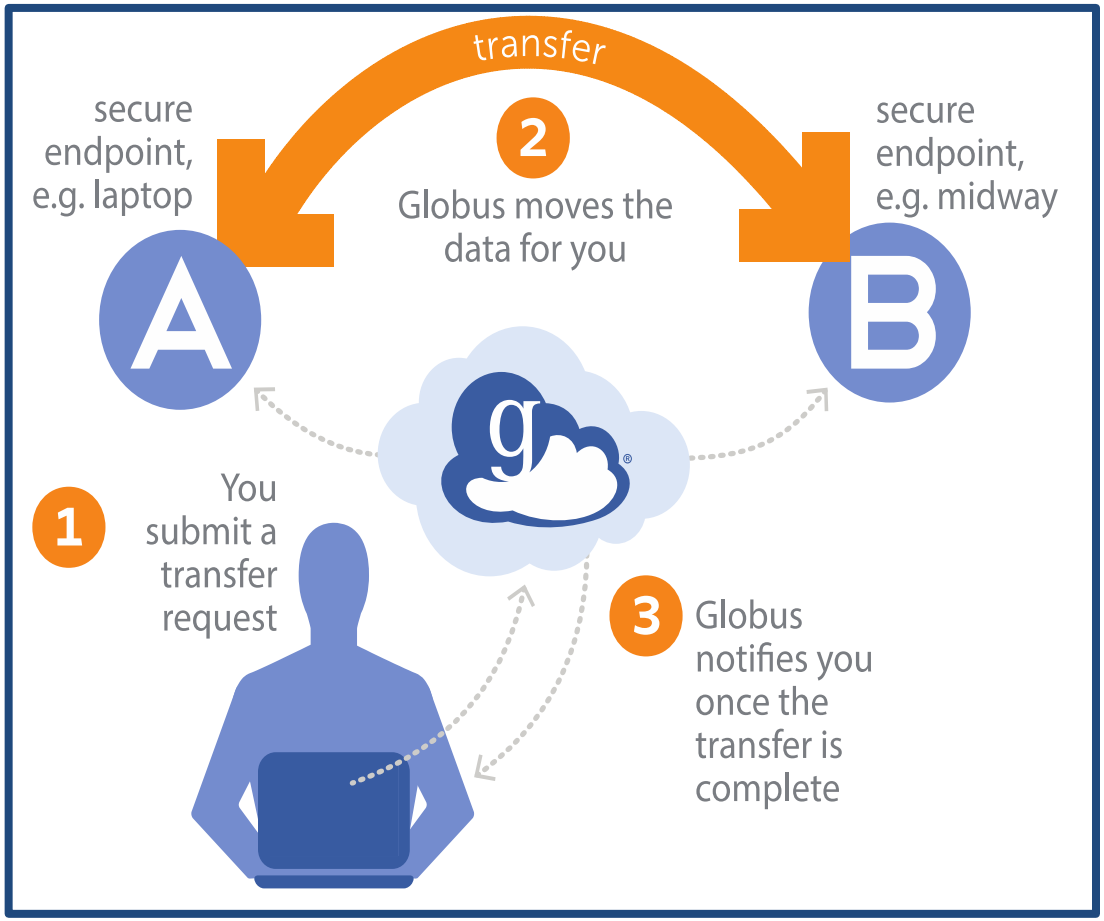
Globus Background

Endpoint

- E.g. laptop or server running a Globus client (e.g. Dropbox client)
- Enables advanced file transfer and sharing
- Currently GridFTP, future GridFTP + HTTP

Some Key Features

- REST API for automation and interoperability
- Web UI for convenience
- Optimizes and verifies transfers
- Handles auto-restarts



313,101,618,927 MB TRANSFERRED

Globus Platform-as-a-Service (PaaS)

Identity management

- create and manage a unique identity linked to external identities for authentication

User groups

- Manage user group creation and administration flows
- Share data with user groups

Publication

Discovery

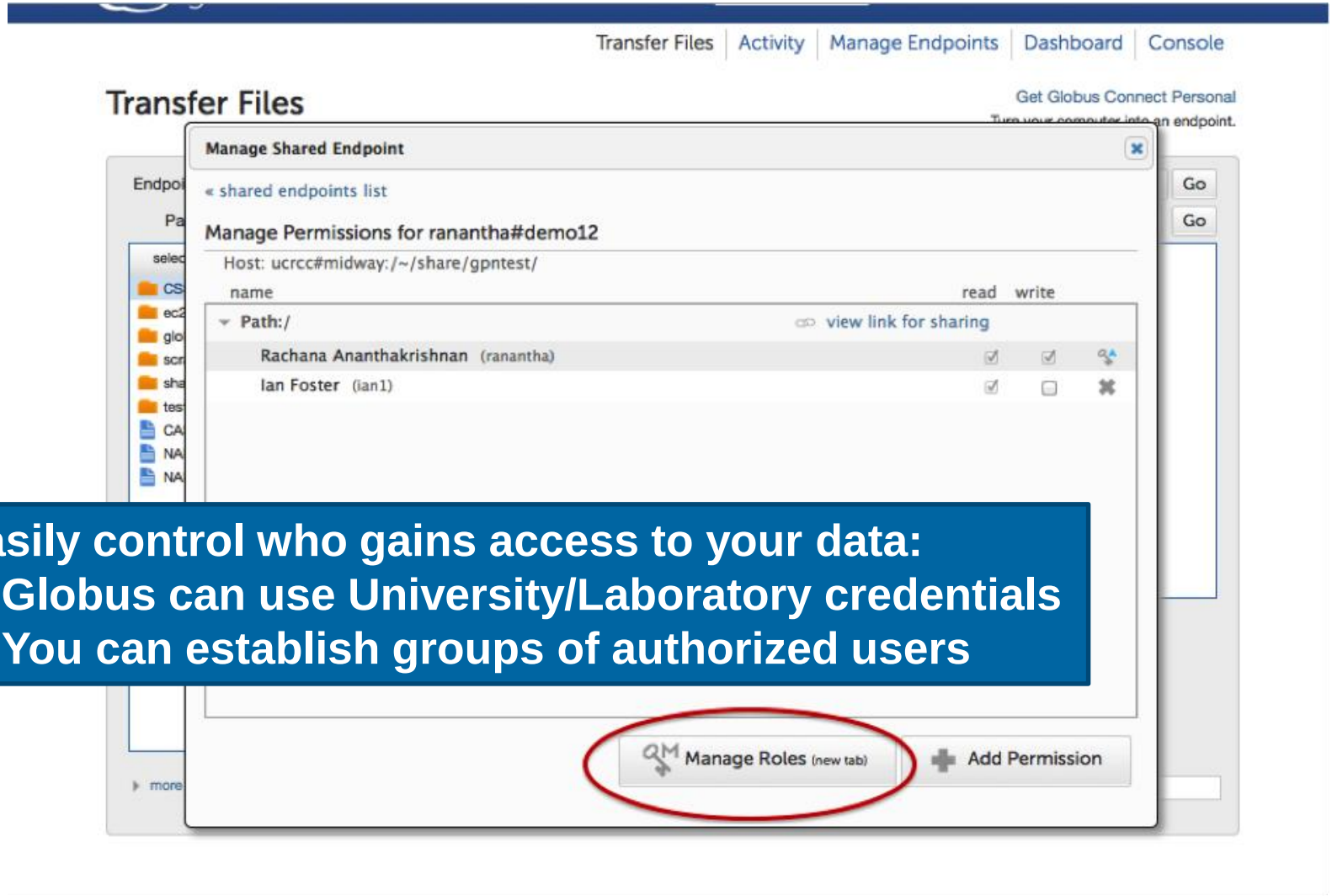
Data transfer

- High-performance data transfer from a web browser
- Optimize transfer settings and verify transfer integrity
- Add your laptop to the Globus cloud with Globus Connect Personal

Data sharing

- Share directly from your storage device (laptop or cluster)
- File and directory-level ACLs

Data sharing and Globus



Easily control who gains access to your data:

- **Globus can use University/Laboratory credentials**
- **You can establish groups of authorized users**

REST APIs, Clients, and Docs

- New Python SDK available
  - https://github.com/globusonline/globus-sdk-python
- Jupyter Notebook Examples
  - https://github.com/globus/globus-jupyter-notebooks
- Sample Data Portal
  - https://github.com/globus/globus-sample-data-portal
- (alpha) MDF Data Publication Service API

Endpoint search

Globus has over 8000 registered endpoints. To find endpoints of interest you can access powerful search capabilities via the SDK. For example, to search for a given string across the descriptive fields of endpoints (names, description, keywords):

```
search_str = "Globus Tutorial Endpoint"
endpoints = tc.endpoint_search(search_str)
print("==== Displaying endpoint matches for search: '{}' ===".format(search_str))
for ep in endpoints:
    print("{} ({})".format(ep["display_name"] or ep["canonical_name"], ep["id"]))
```

Restricting search scope with filters

There are also a number of default filters to restrict the search for 'my-endpoints', 'my-gcp-endpoints', 'recently-used', 'in-use', 'shared-by-me','shared-with-me')

```
search_str = None
endpoints = tc.endpoint_search(
        filter_fulltext=search_str, filter_scope="recently-used")
for ep in endpoints:
    print("{} ({})".format(ep["display_name"] or ep["canonical_name"], ep["id"]))
```

Endpoint details

You can also retrieve complete information about an endpoint, including name, owner, location, and server configurations.

```
endpoint = tc.get_endpoint(tutorial_endpoint_1)
print("Display name:", endpoint["display_name"])
print("Owner:", endpoint["owner_string"])
print("ID:", endpoint["id"])
```

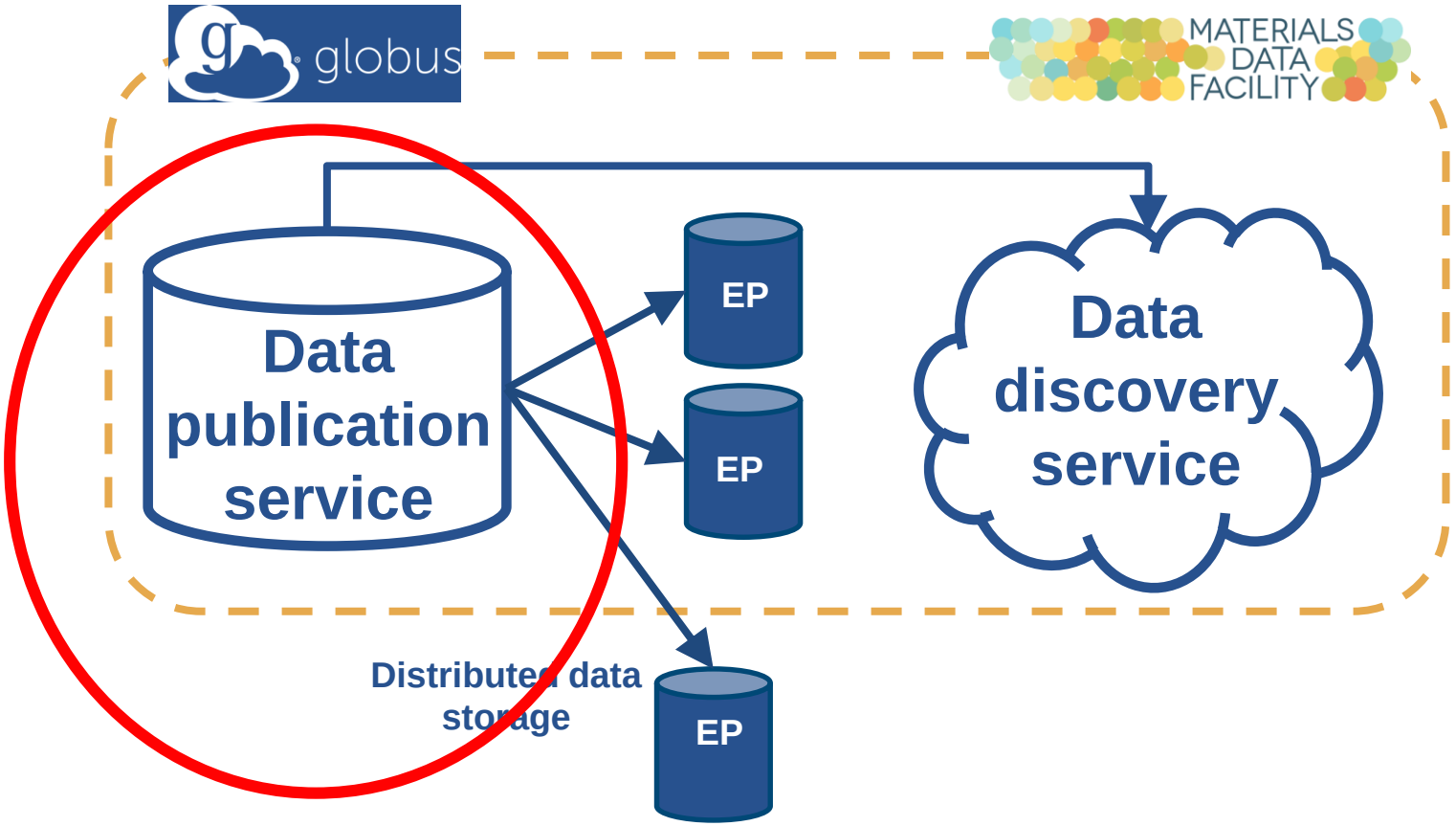
Transfer

Creating a transfer is a two stage process. First you must create a description of the data you want to transfer (which also creates a unique submission_id), and then you can submit the request to Globus to transfer that data.

If the submit_transfer fails, you can safely resubmit the same transfer_data again. The submission_id will ensure that this transfer request will be submitted once and only once.

```
# help(tc.submit_transfer)
source_endpoint_id = tutorial_endpoint_1
source_path = "/share/godata/"

dest_endpoint_id = tutorial_endpoint_2
dest_path = "/~/"

label = "My tutorial transfer"

# TransferData() automatically gets a submission_id for once-and-only-once submission
tdata = globus_sdk.TransferData(tc, source_endpoint_id,
                                dest_endpoint_id,
                                label=label)

## Recursively transfer source path contents
tdata.add_item(source_path, dest_path, recursive=True)

## Alternatively, transfer a specific file
# tdata.add_item("/source/path/file.txt",
#                "/dest/path/file.txt"))

# Ensure endpoints are activated
tc.endpoint_autoactivate(source_endpoint_id)
tc.endpoint_autoactivate(dest_endpoint_id)

submit_result = tc.submit_transfer(tdata)
print("Task ID:", submit_result["task_id"])
```

DATA PUBLICATION



Materials Data Publication Service

MDF Open Collection home page

Open collection for submission of materials-related datasets

Submit to This Collection

Browse

Issue Date | Author | Title | Subject

Datasets in Collection (sorted by Submit Date in Descending order): 1 to 20 of 25

next >

Issue Date	Title	Author(s)
22-Sep-2017	**Dataset for A New Generation of Effective Core Potentials for Correlated Calculations**	*Bennett, M. Chandler; Melton, Cody A.; Annaberdiyev, Abdulgani; Wang, Guangming; Shulenburger, Luke; Mitas, Lubos*
11-Sep-2017	**Probing the growth and melting pathways of a decagonal quasicrystal in real-time**	*Han, Insung; Xiao, Xianghui; Shahani, Ashwin J.*
6-Sep-2017	**Simulated microstructures of gamma' precipitates in cobalt-based superalloys**	*Jokisaari, Andrea M.; Naghavi, Shahab; Wolverton, Chris; Voorhees, Peter W.; Heinonen, Olle G.*
23-Aug-2017	**Solute transport database in Mg using ab initio and exact diffusion theory**	*Agarwal, Ravi; Trinkle, Dallas R.*
29-Jun-2017	**Characterizing the Unifying Thread in High Temperature Superconductors Using Realistic Simulations**	*Narayan, Awadhesh; Busemeyer, Brian; Wagner, Lucas K.*

Datasets Are Citable

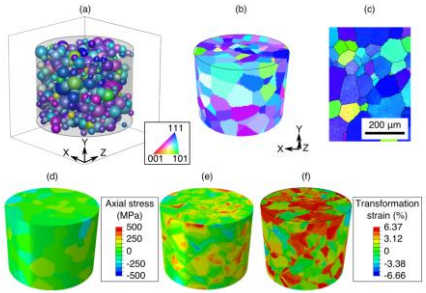
Title 1–20	Cited by	Year
Implications of Grain Size Variation in Magnetic Field Alignment of Block Copolymer Blends Y Rokhlenko, PW Majewski, SR Larson, P Gopalan, KG Yager, CO Osuji American Chemical Society		2017
X-ray Scattering Image Classification Using Deep Learning B Wang, K Yager, D Yu, M Hoai Applications of Computer Vision (WACV), 2017 IEEE Winter Conference on, 697-704	1	2017
Dataset of synthetic x-ray scattering images for classification using deep learning KG Yager, J Lhermitte, D Yu, B Wang, Z Guan, J Liu Materials Data Facility	1	2017
Magnetic field alignment of coil-coil diblock copolymers and blends via intrinsic chain anisotropy Y Rokhlenko, P Majewski, S Larson, K Yager, P Gopalan, A Avgeropoulos, ... Bulletin of the American Physical Society 62		2017

Publication statistics

Data Volumes	**15.0 TB** **13.4 TB out**		
Publication	**50** Total datasets		**16** CHiMaD datasets
	94 Authors	**14** Institutions	**>1000** Accesses
Pipeline	**+30** Total datasets		**+14** CHiMaD datasets

Publication Route #1: MDF Storage

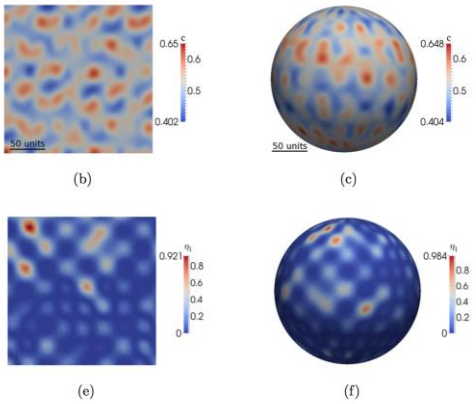
Grain Structure, Grain-averaged Lattice Strains, and Macro-scale Strain Data for Superelastic Nickel-Titanium Shape Memory Alloy Polycrystal Loaded in Tension



- Largest dataset to date (>1.5 TB). Showcases MDF unique capabilities and makes a unique dataset discoverable for code development, analysis, and benchmarking

Paranjape et al.

Phase Field Benchmark I Dataset



Jokisaari et al.

Electron Backscattering and Diffraction Datasets for Ni, Mg, Fe, Si

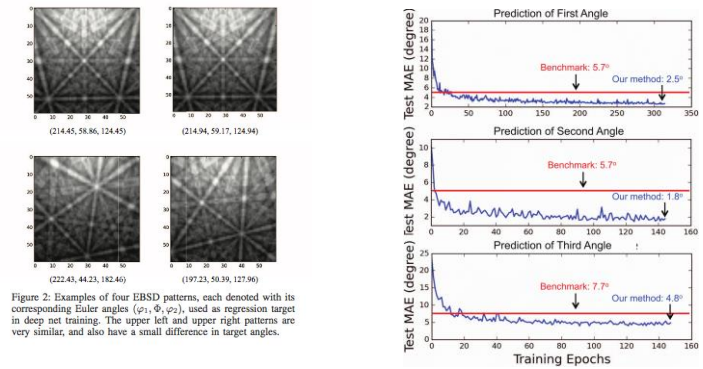
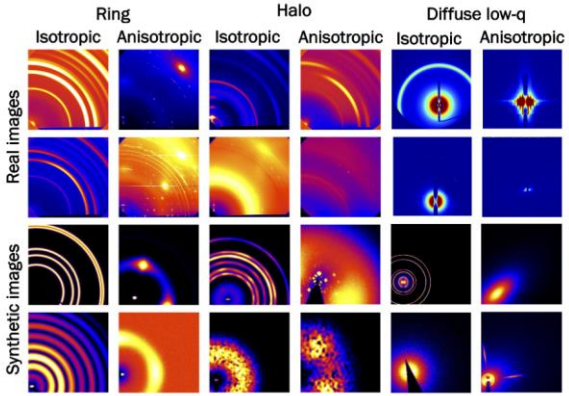


Figure 2: Examples of four EBSD patterns, each denoted with its corresponding Euler angles $(\varphi_1, \Phi, \varphi_2)$, used as regression target in deep net training. The upper left and upper right patterns are very similar, and also have a small difference in target angles.

Marc De Graef et al.

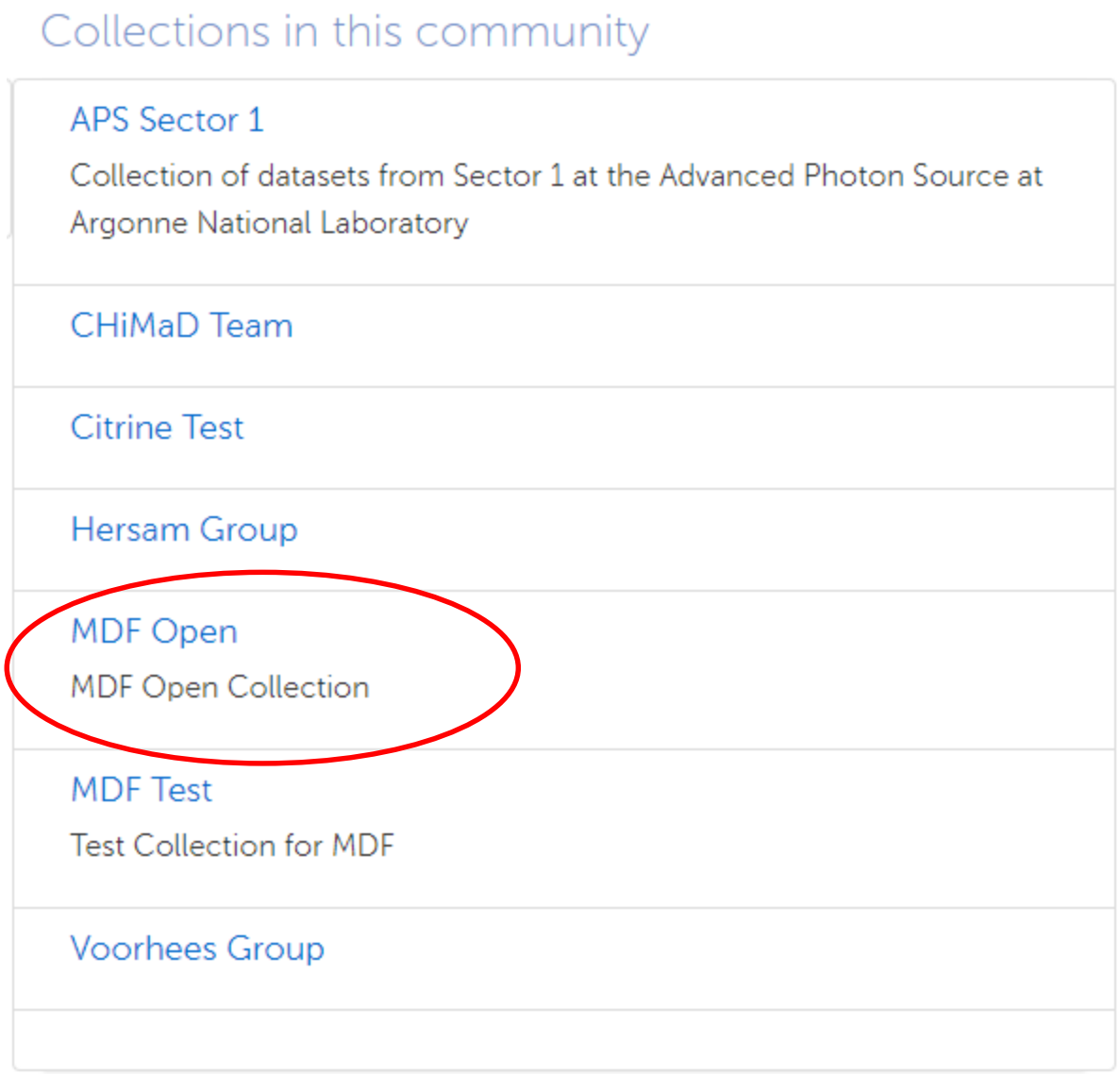
X-ray Scattering Image Classification Using Deep Learning



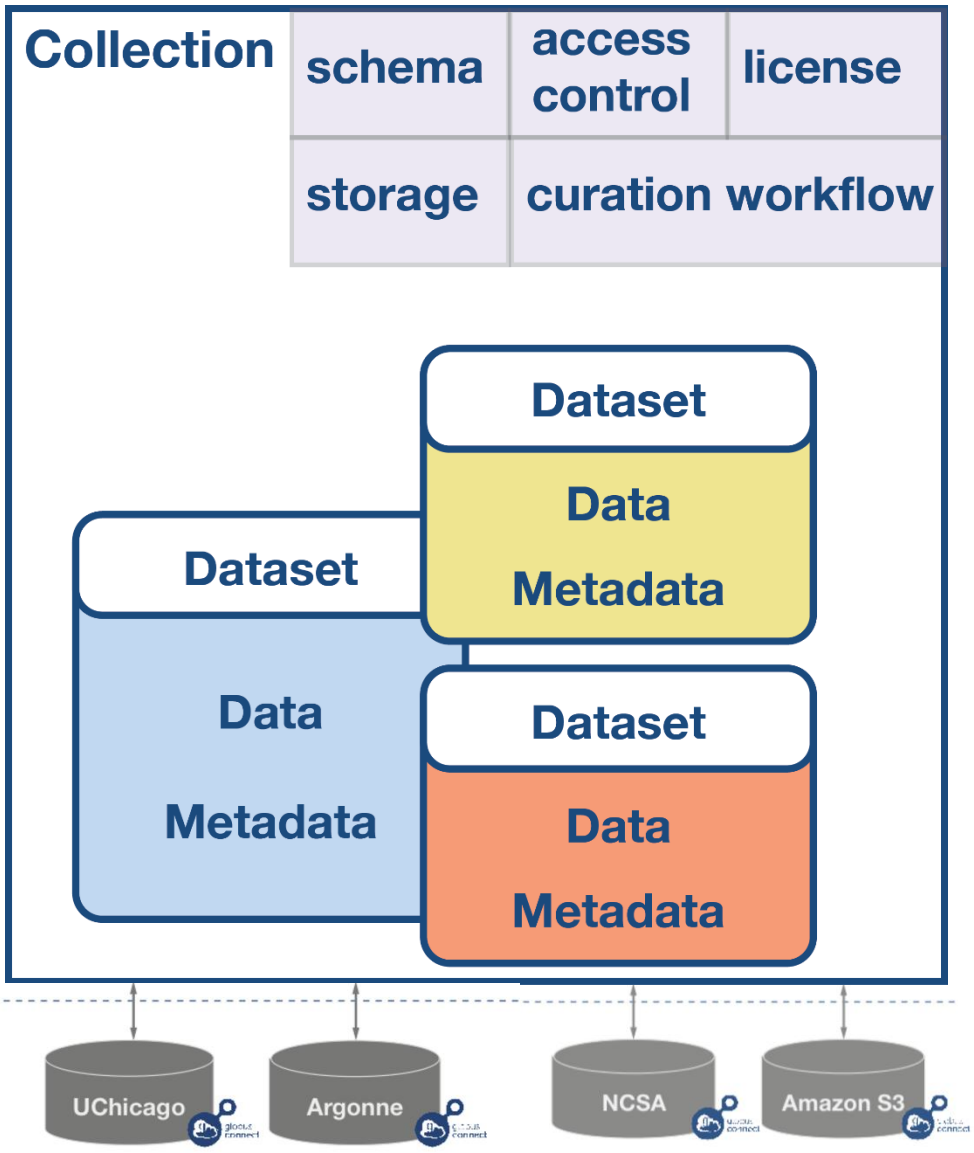
layer name	output size	kernels
conv1	112×112	7×7, 64, stride 2
		3×3 max pool, stride 2
conv2_x	56×56	$\begin{bmatrix} 1\times1, 64 \\ 3\times3, 64 \\ 1\times1, 256 \end{bmatrix} \times 3$
conv3_x	28×28	$\begin{bmatrix} 1\times1, 128 \\ 3\times3, 128 \\ 1\times1, 512 \end{bmatrix} \times 4$
conv4_x	14×14	$\begin{bmatrix} 1\times1, 256 \\ 3\times3, 256 \\ 1\times1, 1024 \end{bmatrix} \times 6$
conv5_x	7×7	$\begin{bmatrix} 1\times1, 512 \\ 3\times3, 512 \\ 1\times1, 2048 \end{bmatrix} \times 3$
pooling	1×1	average pooling
fc	1×1	2048×num of attributes

Yager et al. http://dx.doi.org/10.18126/M2Z30Z

Customization: Collection Model



Customization: Collection Model



- **Collections might be a research group or a research topic...**
- **Collections have specified**
  - Mapping to storage endpoint
    - Currently handled as automatically created shared endpoints
  - Metadata schemas
  - Access control policies
  - Licenses
  - Curation workflows
- **Collections contain**
  - Datasets
    - Data
    - Metadata
- **Metadata Persistence**
  - Metadata log file with dataset
  - Metadata replicated in search inde

Share Data with Flexible ACLs

- Share data publicly, with a set of users, or keep data private

Leverage Curation Workflows

- Collection administrators can specify the level of curation workflow required for a given collection e.g.
  - No curation
  - Curation of metadata only
  - Curation of metadata and files

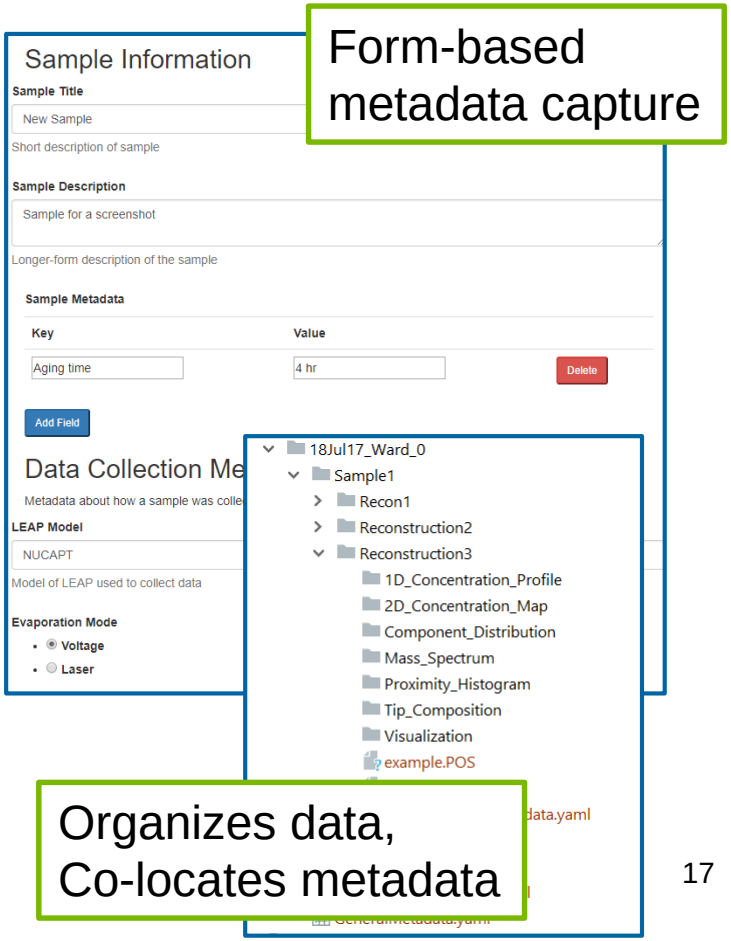
Example: NUCAPT Data Publication

MATERIALS DATA FACILITY

Goal:
- Aid metadata capture
- Simplify data publication

Approach: Lightweight web service
- Form-based metadata capture
- Automatic file management
- "One-click" data publication

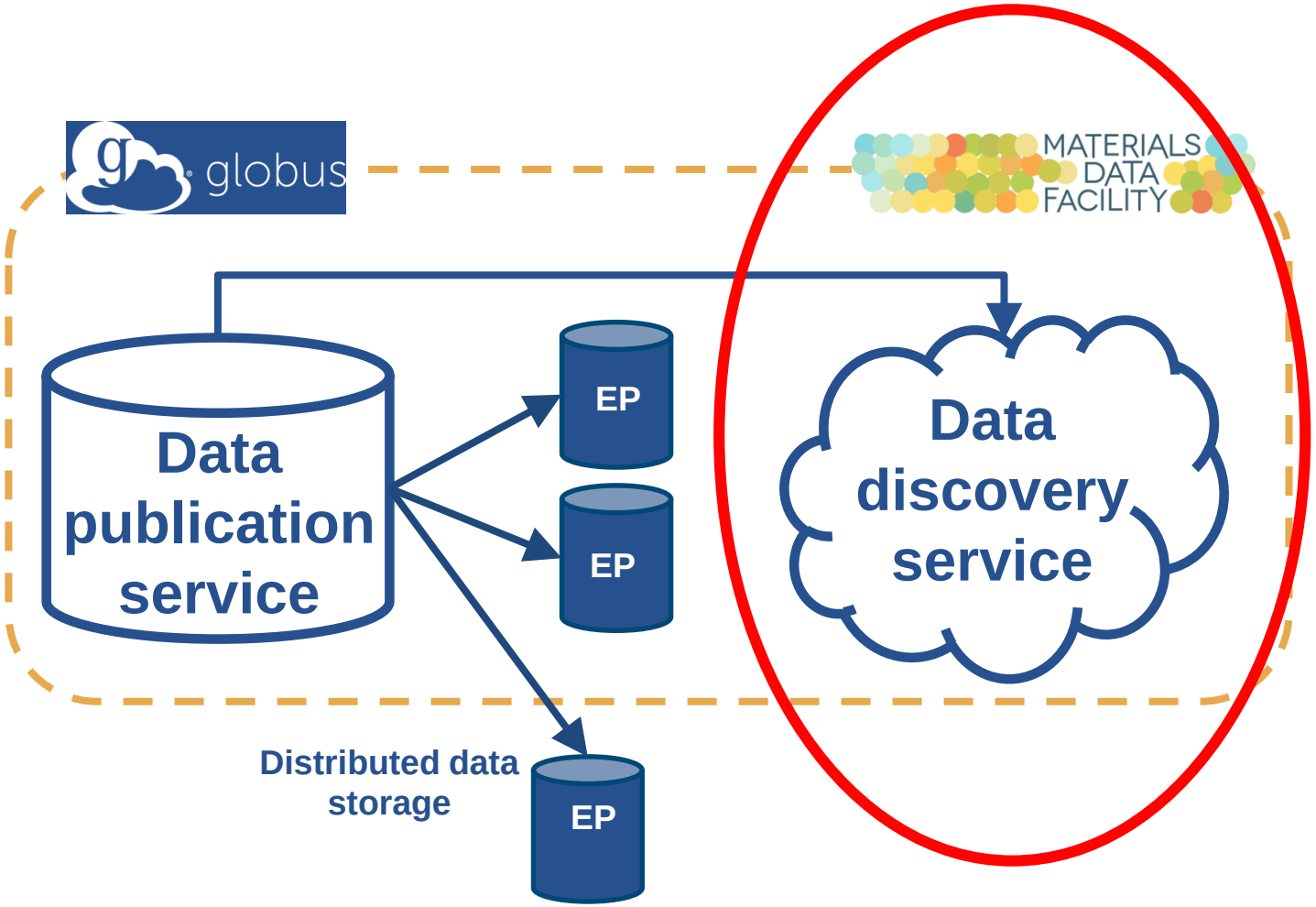
Results:
- Beta version deployed Sept '17



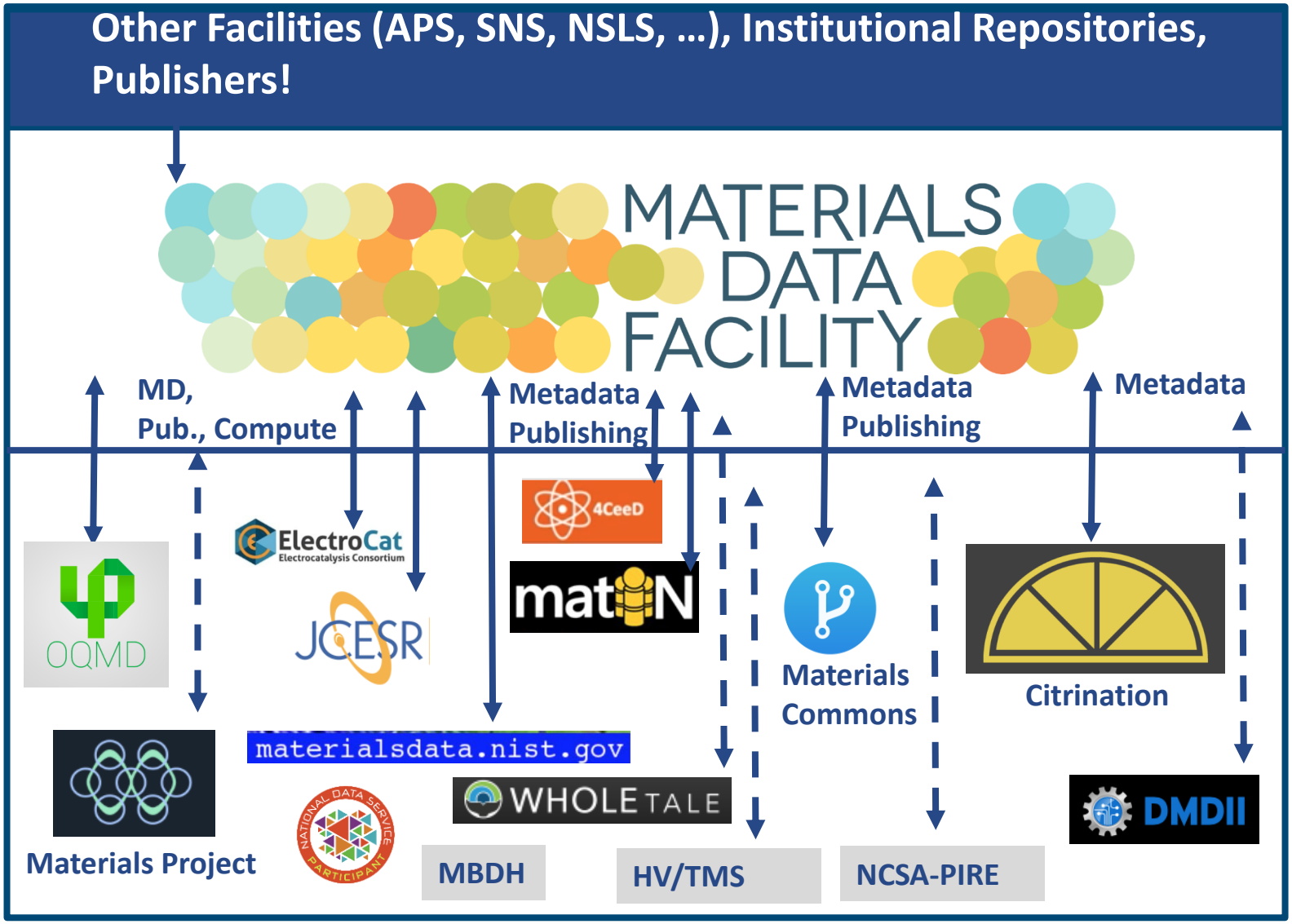
Form-based metadata capture

Organizes data, Co-locates metadata

DATA DISCOVERY [AND USE]

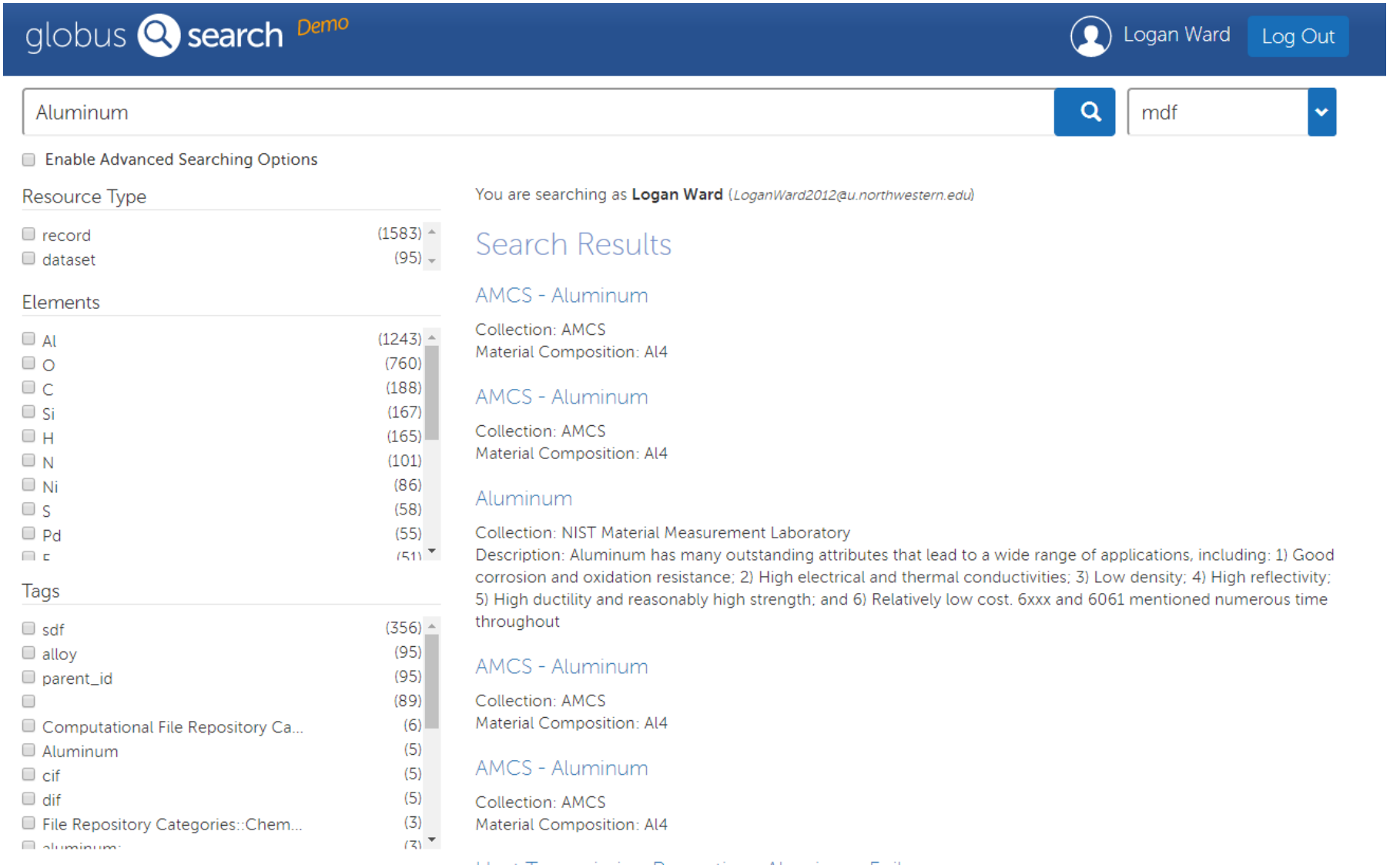


Part 1: Linking with the Data Community



zenodo MICCoM NOMAD The Dataverse Project

Many Databases, Single Search



MDF + NIST Database Tools

Querying Nanomine Data

Example using the Materials Data Facility to query data from NanoMine

```
In [1]: from mdf_forge.forge import Forge
```

Get All Records

Get all of the records in NanoMine

```
In [2]: forge = Forge()

In [3]: data = forge.search('mdf.source_name=nanomine AND mdf.resource_type=record', advanced=True)

In [4]: print('Found %d records in NanoMine'%len(data))

Found 227 records in NanoMine
```

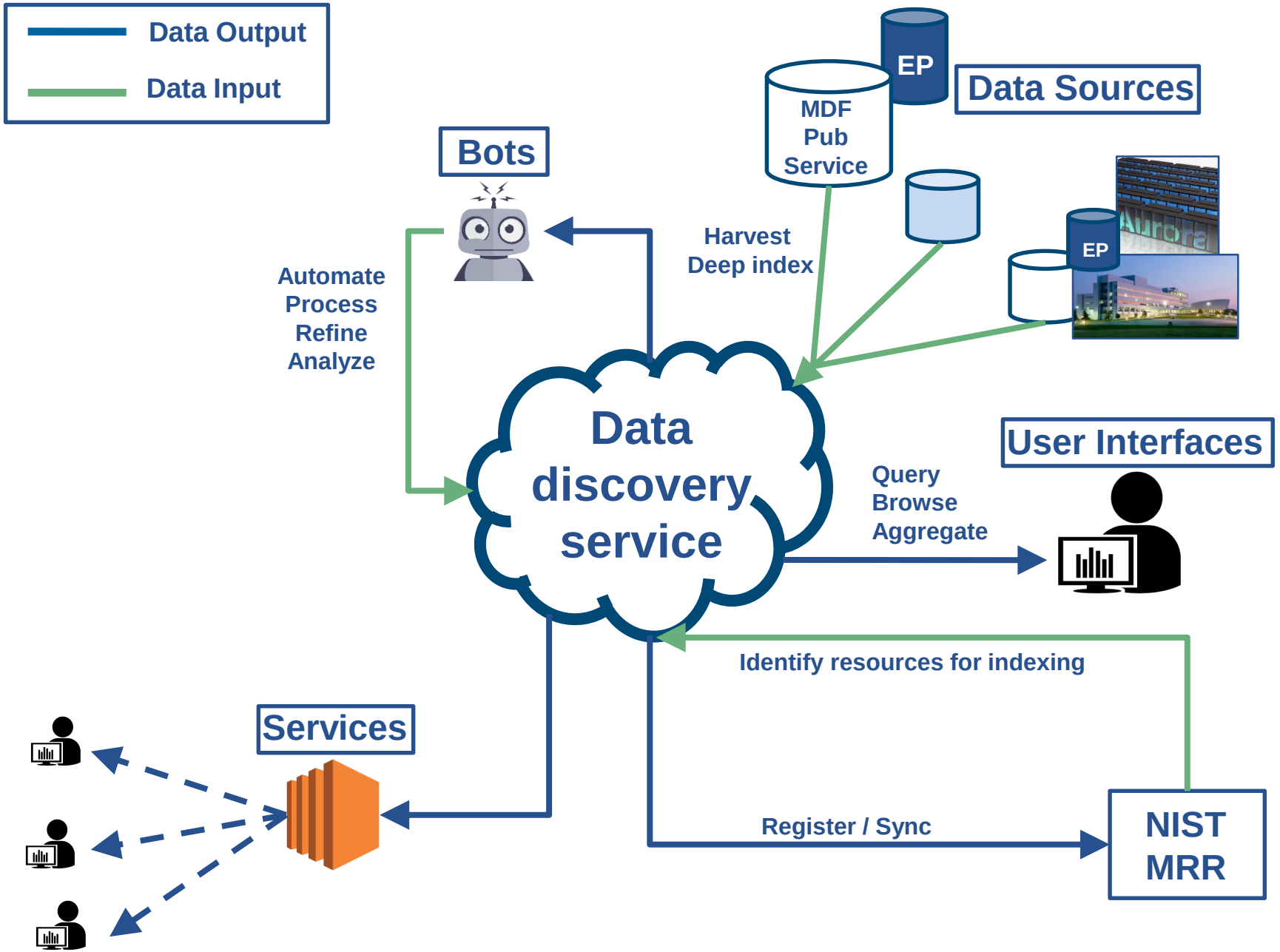
MDF automates publicizing data and provides a uniform search interface

Get Records with Olefin Matrices

Example of a more-complex query

```
In [5]: data = forge.search('mdf.source_name=nanomine AND '
                            'content.PolymerNanocomposite.MatrixComponent.ChemicalName=olefin', advanced=True)

In [6]: print('Found %d olefin records'%len(data))

Found 6 olefin records
```

MDF data discovery ecosystem



Summary

Three Major Components of Materials Data Facility

1. Globus
   - High speed data transfer
   - Easy data sharing
2. Data Publication Service
   - Simple data publication, from your own
   - Free data publication
3. Data Discovery Service
   - Single search engine for many materials databases
   - Python API for accessing these databases

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