

#### **The Materials Data Facility**

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materialsdatafacility.org





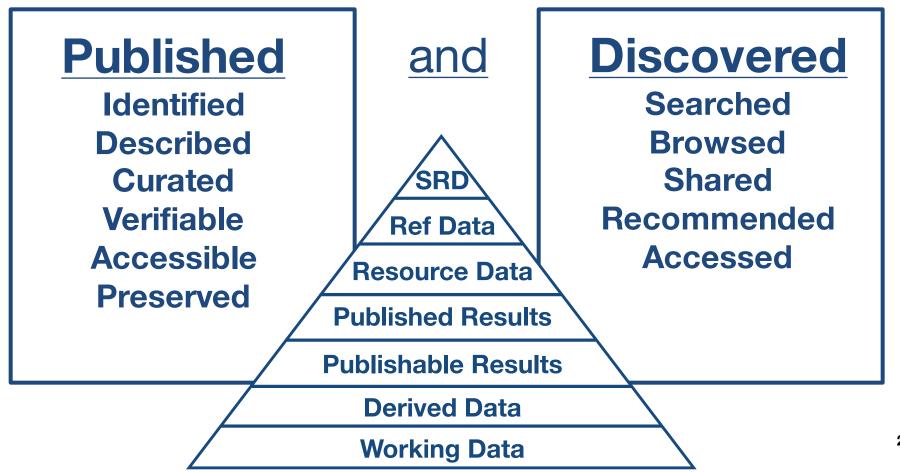






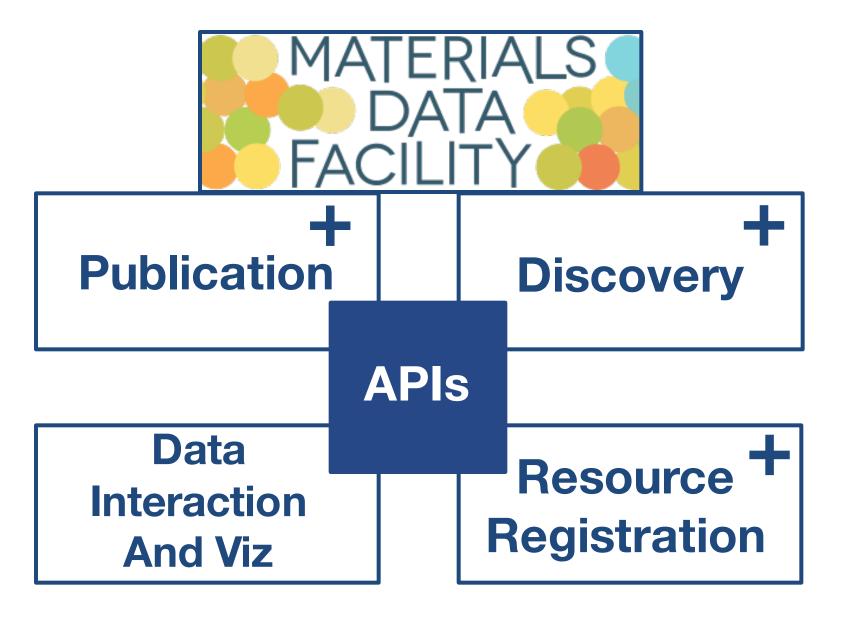
#### What is MDF?

## We aim to make it simple for materials datasets and resources to be ...



# What infrastructure do we need to effectively support materials researchers?

#### **Service Infrastructure**



#### **Publication**

#### **Deployed Nov. 2015**

- Identify datasets with persistent identifiers (e.g. DOI)
- <u>Describe</u> datasets with appropriate metadata, and provenance
- Curate dataset metadata and data composition
- Verify dataset contents over time
- <u>Preserve</u> critical datasets in a state that increases transparency, replicability, and helps encourage reuse

#### **Discovery**

#### **Coming late 2016-ish**

- Search and query datasets in modern ways e.g. via indexed metadata rather than remembering file paths
- Discover distributed materials resources (more later)



## Resource Registration

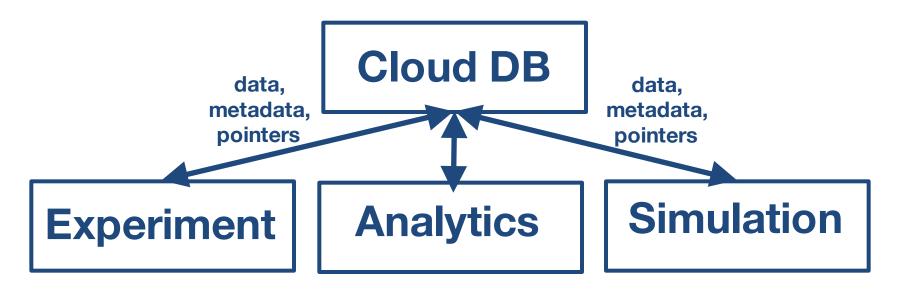
## Coming Q1 2016 via NIST

- Find existing, widely distributed, materials resources
- Register new resources into the network



## Data Interaction And Viz

- Data-driven experiments using HPC resources and workflow technologies
- Real-time interaction with data regardless of data location (pending appropriate data access) and data size
- (future) Machine learning across datasets and storage locations
- (future) Automated discovery support



#### **Understanding Incentives is Critical**

#### Increasing Impact

- Increase paper citations<sup>1</sup>
- Add dataset citation capabilities

## Meeting Award Requirements

Simplify DMP compliance

### Smoothing Dislocations

- Enable simple sharing among collaborators (near and far)
- Ease transitions between students
- Lessen need for ad hoc resource sharing (e.g. via group websites)

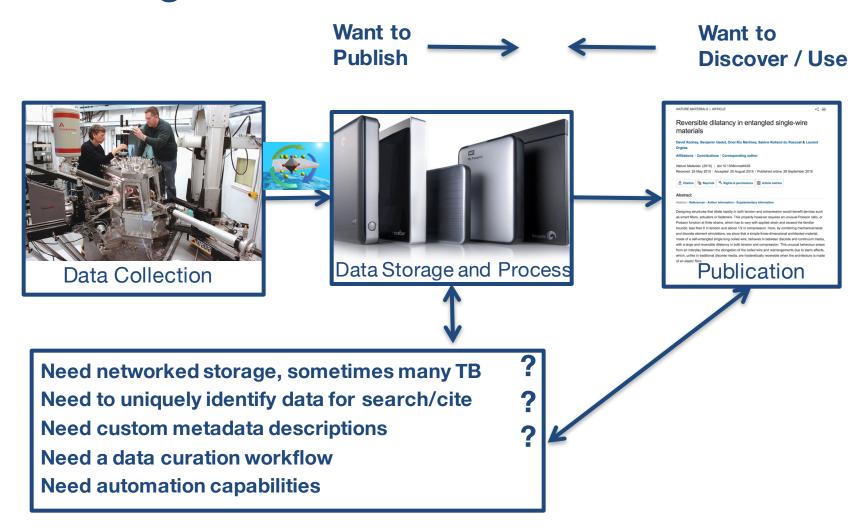
## So where are we now?

Publication

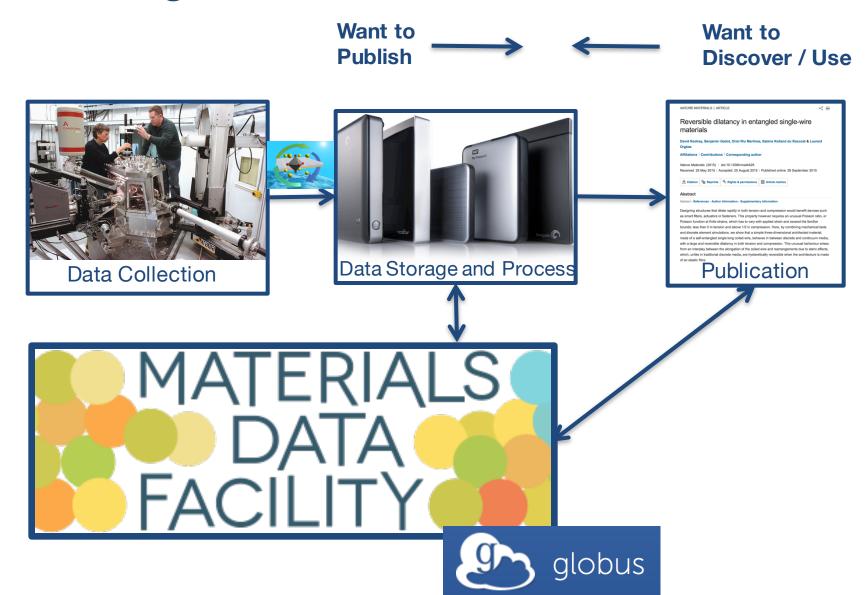
## Materials Data Publication/Discovery is Often a Challenge



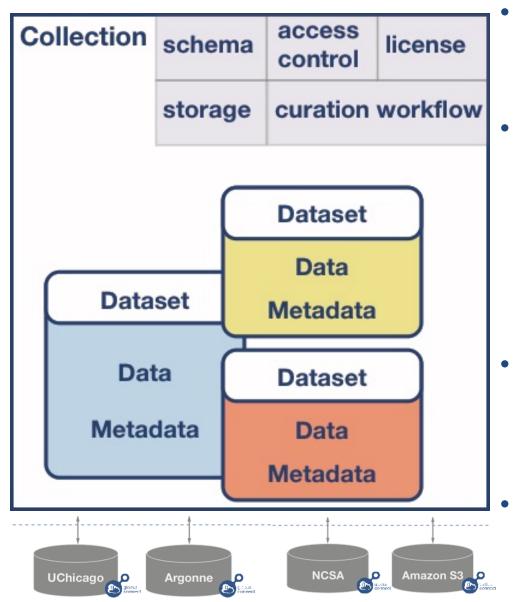
## Materials Data Publication/Discovery is Often a Challenge



## Materials Data Publication/Discovery is Often a Challenge



#### **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 index

#### **Publish Large Datasets**

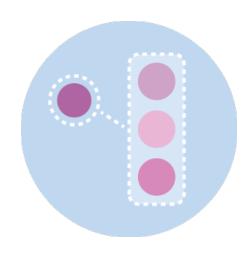


 Leverages Globus production capabilities for file transfer, user authentication, and groups

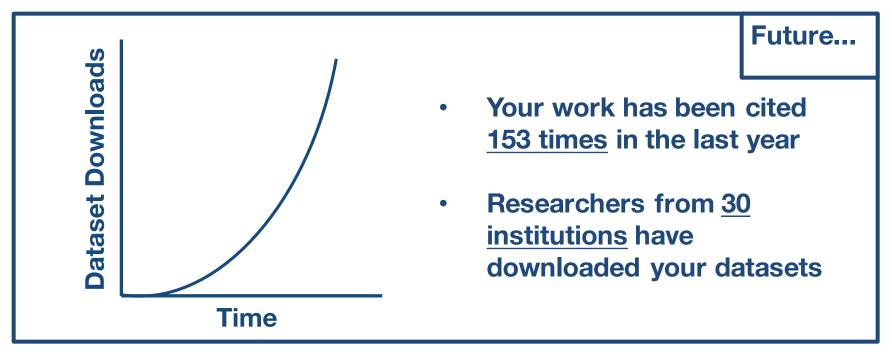
127,289,944,744 MB TRANSFERRED

- 100 TB of reliable storage @ NCSA, and more storage at Argonne
  - Globus endpoint at ncsa#mdf
  - Expandable to PBs as necessary
  - Automated tape backup for reliability (in progress)
- Optionally use your own local or institutional storage

#### **Uniquely Identify Datasets**



- Associate a unique identifier with a dataset
  - DOI, Handle
- Improve dataset discovery and citability
  - Aligning incentives and understanding the culture will be critical to driving adoption



#### **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

#### **Customize Metadata**



- Build a custom metadata schema for your specific research data
- Re-use existing metadata schemas
- Working in conjunction with NIST researchers to define these schemas

#### Future...

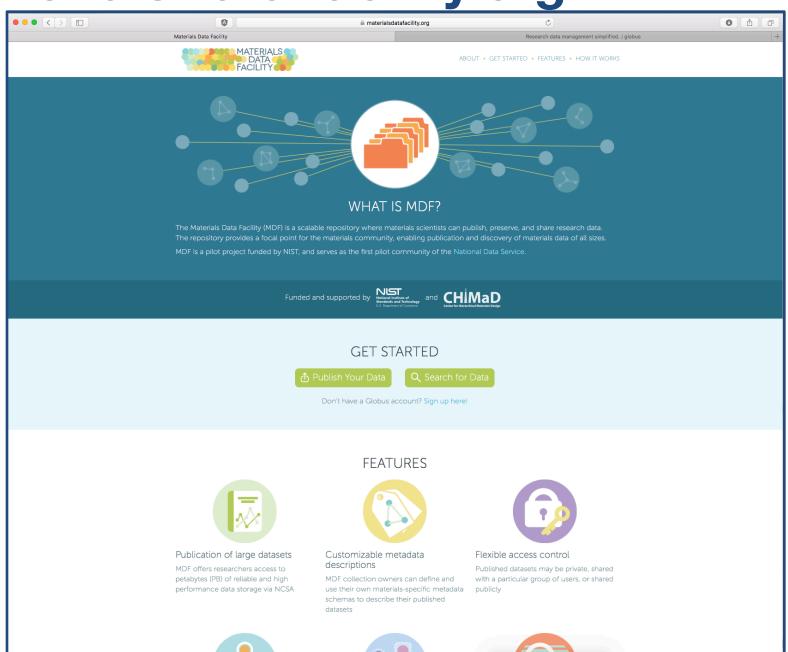
- Can we build a system that allows schema:
  - Inheritance
    - E.g. a schema "polymers" might inherit and expand upon the "base material" of NIST
  - Versioning
    - E.g. Understand contextually how to map fields between versions
  - Dependence
    - E.g. Allows the ability to build consensus around schemas

#### **Discover Research Datasets**



- Search on file metadata, custom metadata, and indexed file-level data
- Goal: Intuitive search (e.g. Google-style)
  with support for more complex range
  queries and faceting (e.g. Amazon-style)

#### **MaterialsDataFacility.org**



## MDF Submission Walkthrough

#### **Example Use Case**

#### **Publishing Big, Remote Data**

Group has taken <u>50 TB</u> of data <u>at APS</u> need to send back to home inst. For analysis and archiving

**Bundle** multiple experimental runs with metadata and provenance

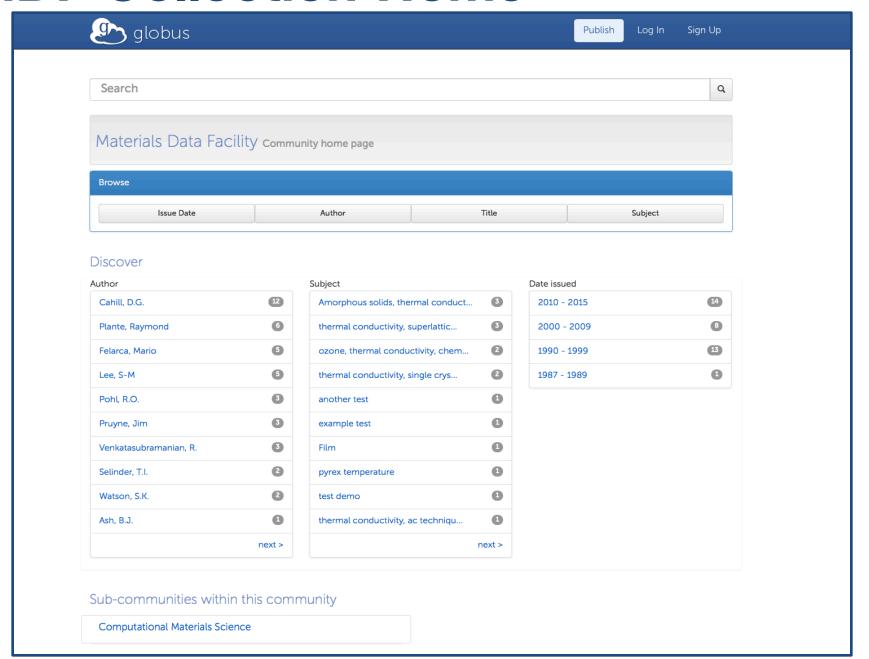
PI wants to <u>verify dataset</u> data/metadata before pub.

Want a <u>citable DOI</u> to share the raw and derived data with the community

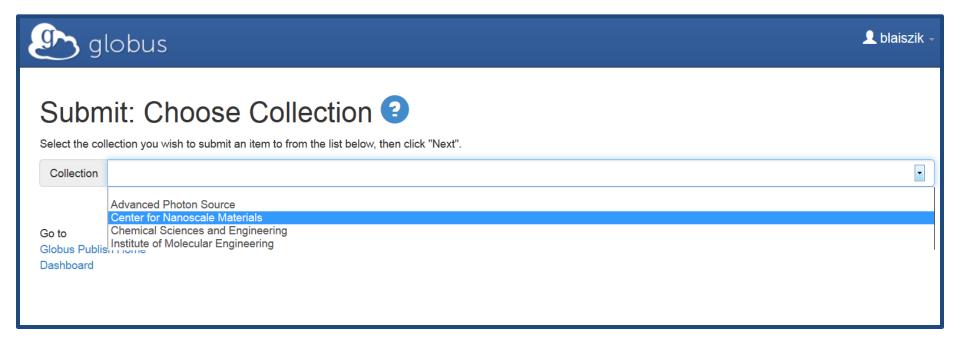
Want their data to be <u>discoverable</u> by free text search and <u>custom</u> metadata



#### **MDF Collection Home**



#### **MDF Collections**

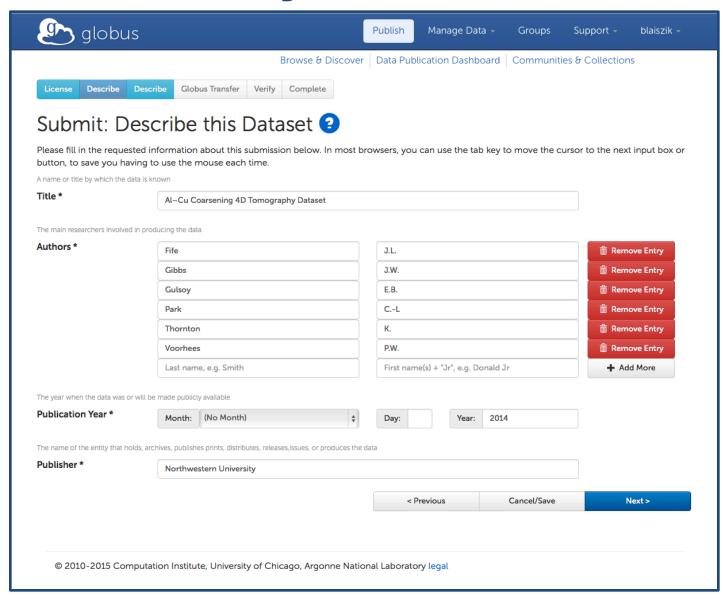


#### Recall: Policies Set at the Collection Level

- Required metadata, schemas
- Data storage location
- Metadata curation policies

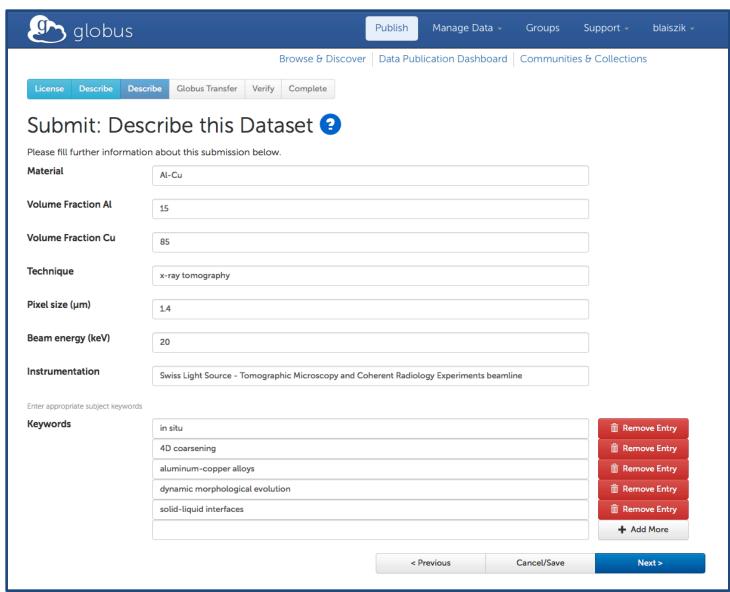
#### **MDF Metadata Entry**

- Scientist or representative describes the data they are submitting
- For this collection Dublin Core and a custom metadata template are required



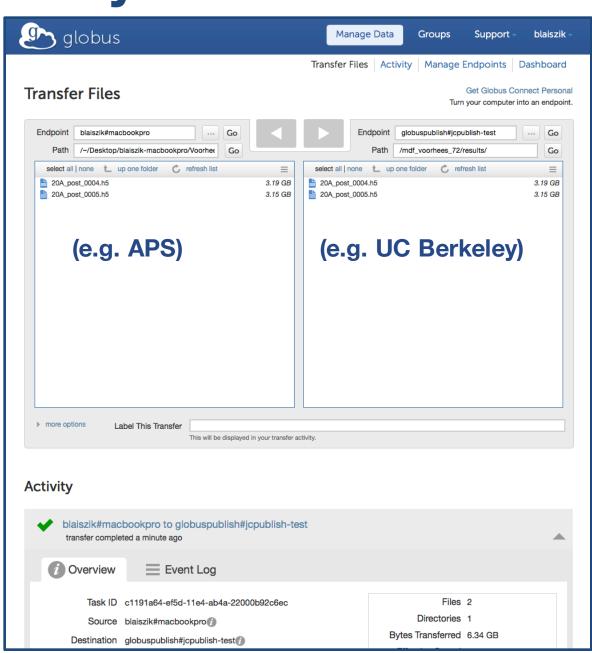
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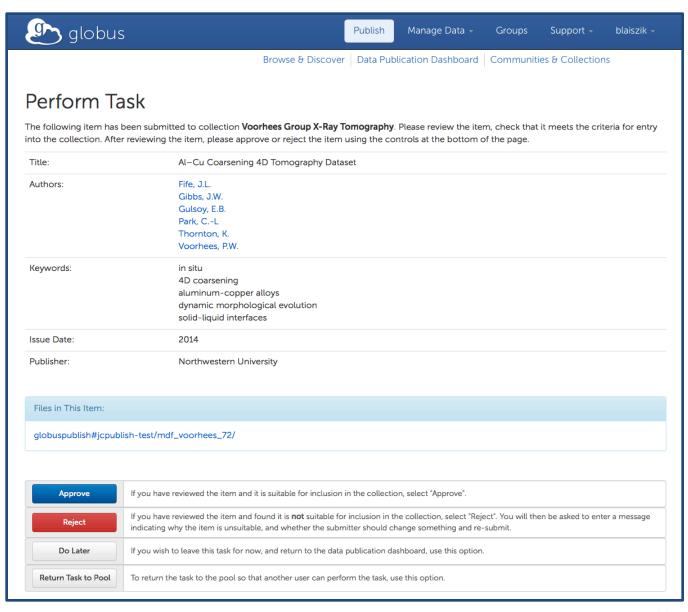
#### **Dataset Assembly**

- Shared endpoint is auto-created on collection-specified data store
- Scientist transfers dataset files to a unique publish endpoint
- Dataset may be assembled over any period of time
- When submission is finished, dataset will be rendered immutable via checksum

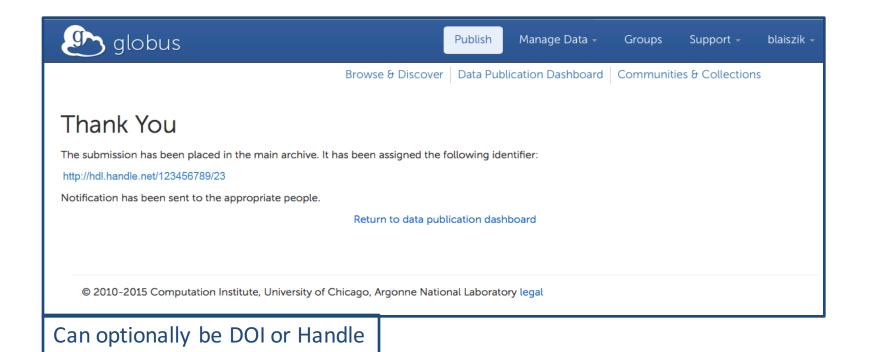


#### **Dataset Curation**

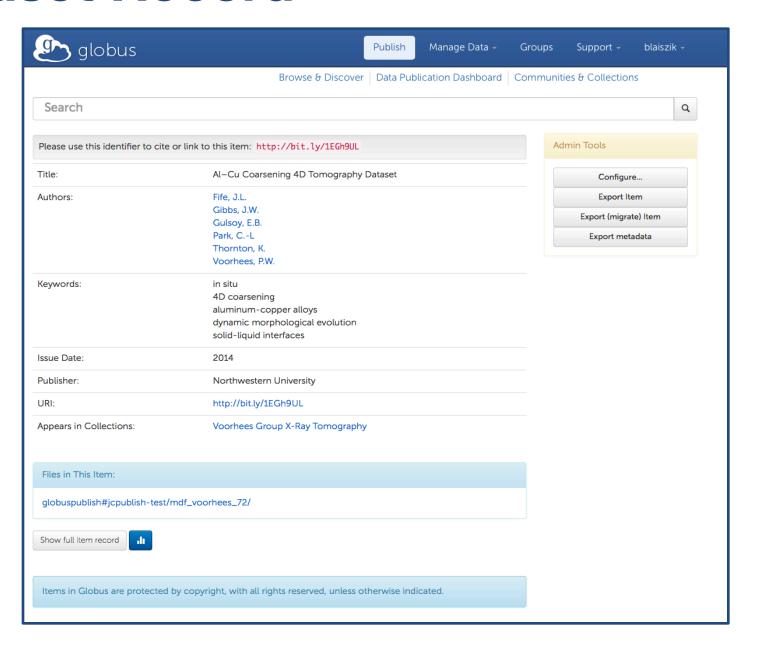
- Optionally specified in collection configuration
- Can be approved or rejected (i.e. sent back to the submitter)



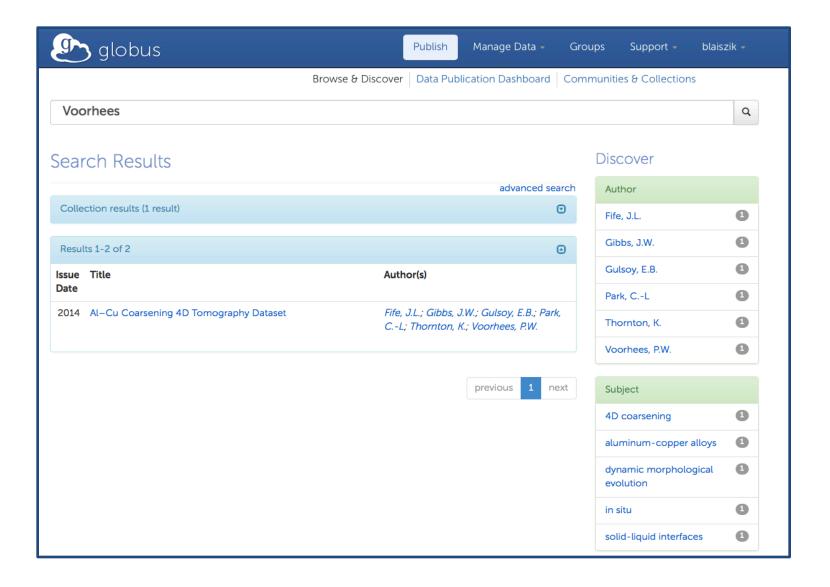
#### Mint a Permanent Identifier



#### **Dataset Record**

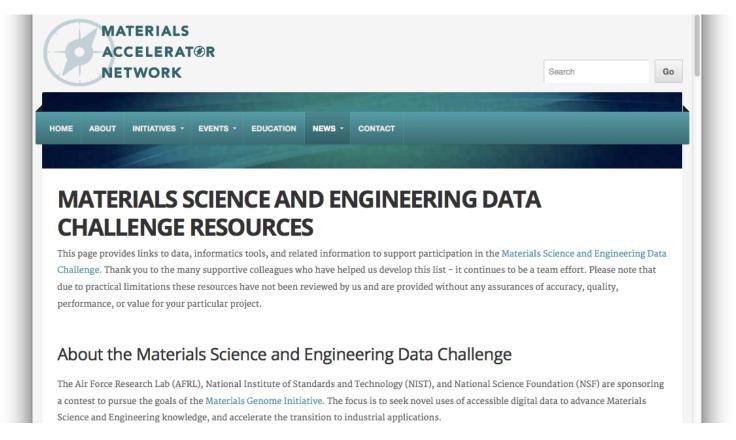


#### **Dataset Discovery**



## Registering Materials Resources

#### **Materials Resource Registry**



http://acceleratornetwork.org/mse-challenge/

#### Materials Science Data Challenge

#### **Materials Resource Registry**

#### **Data Resources**

#### **Computed Data**

AFLOW database

Computational Materials Data (CMD) Network

Harvard Clean Energy Project

Materials Project

National Institute of Standards and Technology (NIST) Interatomic Potentials Repository Project

Open Knowledgebase of Interatomic Models (KIM) or OpenKIM

Open Quantum Materials Database (OQMD)

Experimental (and possibly computed)

Data

3D Materials Atlas

American Mineralogist Crystal Structure

#### **Data Mining Tools**

Best Data Mining Tools by Quora

Citrine. See also their blog posts on machine learning for the materials scientist part 1 and part 2.

Dream3D

Fiji (ImageJ)

Granta (Material Intelligence)

Massive Online Analysis (MOA)

Materials Knowledge Systems in Python (PyMKS)

Matlab

Matlab Toolbox for Dimensionality Reduction by Laurens van der Maaten

nanoHUB

Nutonian Eurega

#### Places to Publish, Share (and Find) Data

#### Journals with Data Focus

Data in Brief (DiB) (Elsevier) . See also Harvard Dataverse DiB section.

#### Harvard Dataverse

Integrating Materials and Manufacturing
Innovation (IMMI) (see Data Descriptor article
type)

#### Materials Discovery (Elsevier)

Open Data journals at Elsevier. Part of a number of projects at Elsevier supporting the Materials Genome Initiative. See also Elsevier's page on their resources for the MS&E Data Challenge.

Scientific Data (Nature Publishing Group)

#### **Data Repositories and Data Sharing Tools**

Citrine (see their blog for details on their support of datasets for the Challenge)

## Materials Accelerator Network

#### **Materials Resource Registry**



me Services »

Dashboard

Help

Conta

1

#### Materials Resource Registry

#### Search Results for 'compound'







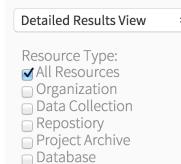






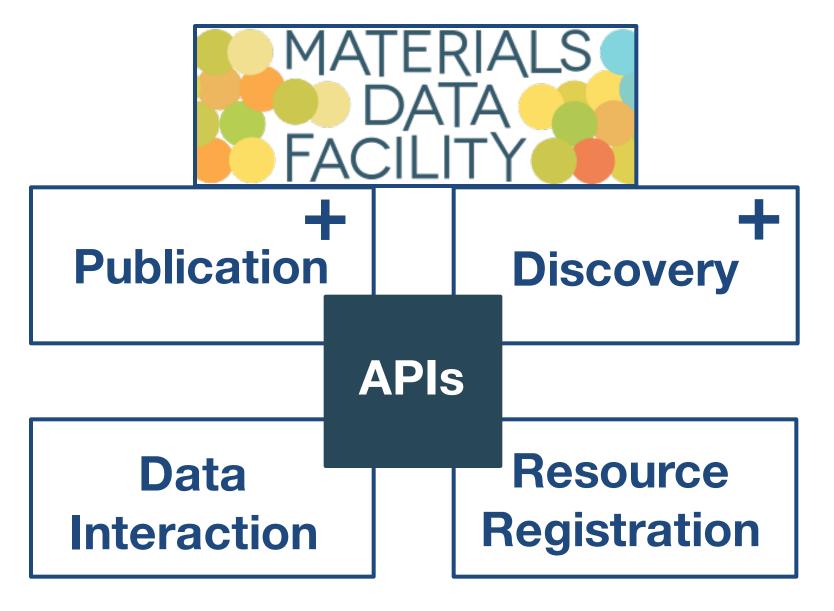








#### **Service Infrastructure**



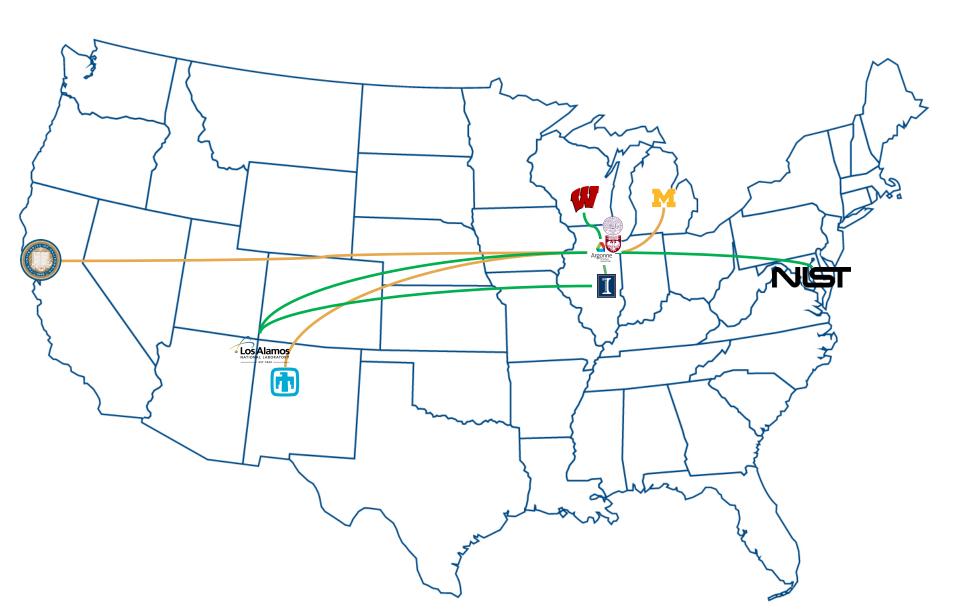
### What's Available?

- Web interface to support data publication via Globus platform (identify management, user groups, optimized big data transfer)
- 100 TB of storage at NCSA (scalable to >1 PB) more at Argonne (?)
- Help with developing metadata schemas to describe your research datasets

# Yet another publication system?

- Software as a Service
- Self service management
  - Identifiers, policies, submission and curation workflows, storage, metadata, access control
- Remote storage
- Supports arbitrarily large datasets
- Powerful search

## **Current Interactions**

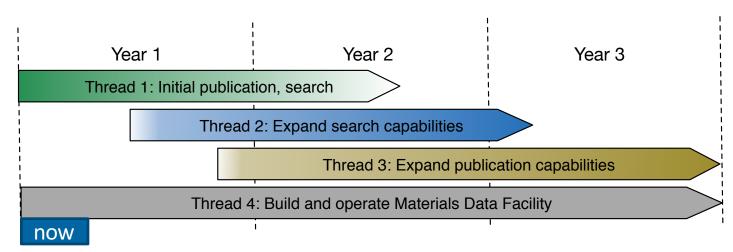


# What are we looking for?

- Early adopters, willing to get their hands dirty with the service and give honest feedback
- Key datasets of all sizes, shapes, raw or derived, that might help us understand the process better

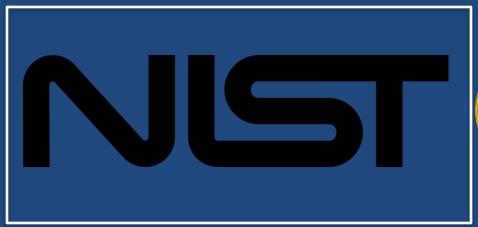
 Currently working with researchers from UIUC, NWU, UC Berkeley, UW-Madison, UMichigan, Argonne

# **Next Steps**



- Identify datasets to pilot publication pipelines and build schema repository
- Engage with researches working with materials data to understand use cases and learn friction points
- Please talk to us if you have data you want to share, publish, discover, ...
- Globus tutorials (identity, transfer, sharing): https://github.com/globusonline/globus-tutorials

# **Thanks to Our Sponsors!**















## Globus delivers...

big data transfer, sharing, publication, and discovery...

...directly from your own storage systems...

...via software-as-a-service

### Globus is SaaS

- Access made easy via Web browser
  - Command line, REST interfaces, python clients for flexible automation and integration

New features automatically available without user updates

- Reduced IT operational costs
  - Small local footprint (Globus Connect)
  - Consolidated support and troubleshooting

# **User Experience**



flickr ...for your photos



Google ...for your office docs



METERIA ... for your entertainment



# Globus Platform-as-a-Service (PaaS)

# **Identity** management

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

# Data publication

# Data

 High-performance data transfer from a web browser

transfer

- Optimize transfer settings and verify transfer integrity
- Add your laptop to the Globus cloud with Globus Connect Personal

# **User** groups

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

# Data sharing

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

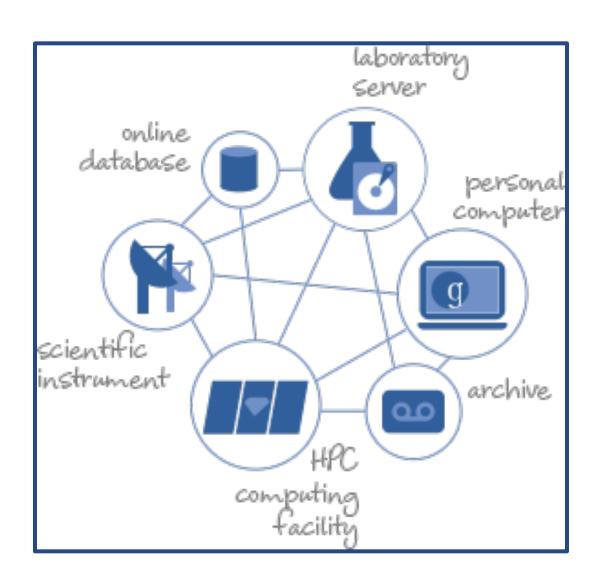
## **Background**

#### **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
- Battle tested with big data



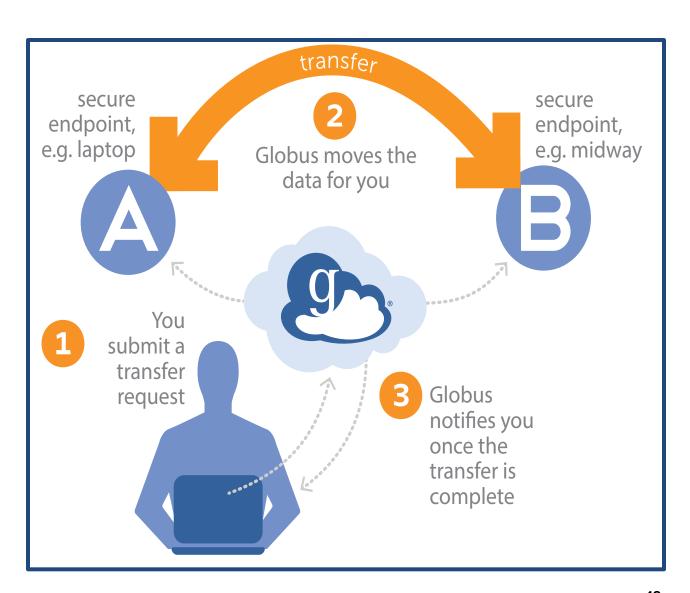
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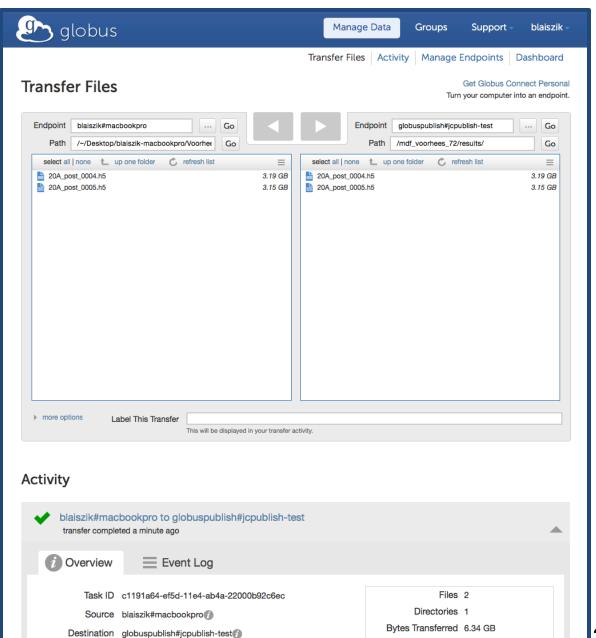
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# **Identity Management**

#### **Key Features**

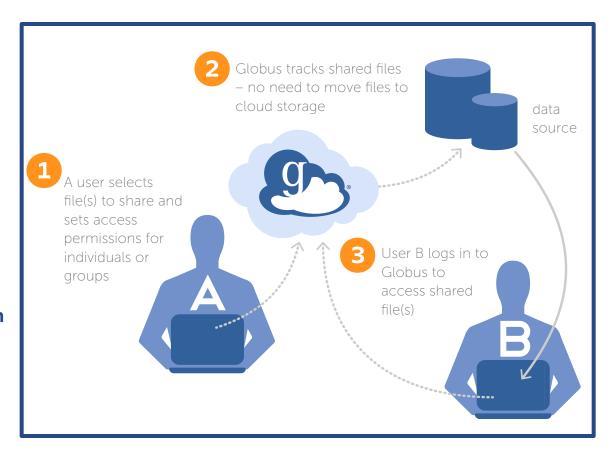
- Leverage institutional credentials
- Link multiple identities
- Standard oAuth2 flow



# **User Groups and Sharing**

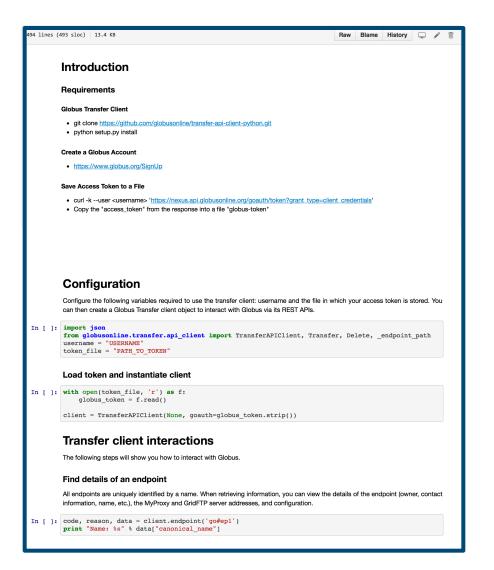
#### **Key Features**

- Share without users requiring accounts on your systems.
- Share data in place, no need to move to the cloud
- Maintain security and access controls as defined by your resource provider.
- Groups: Manage permissions on a group basis rather than on an individual basis



# Globus PaaS Jupyter Notebooks

### https://github.com/globusonline/globus-tutorials



**Identity** management

**User groups** 

Data transfer

Data sharing

### **Create an Account**

- Go to: www.globus.org/signup
- 2. Create your Globus account
- 3. Validate e-mail address
- 4. Optional: Login with your campus/InCommon identity
- 5. Install Globus Connect Personal
- 6. Clone repo
  - git clone https://github.com/globusonline/globustutorials
- 7. Move files from kyle#ncsa-tutorial endpoint to your laptop