

Deployment of NIST Pilots on NDS Labs

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Deployment of NIST Pilots on NDS Labs

Pilots deployed (success stories):

- MGI Code Catalog (December 2015)
- NIST Materials Resource Registry (January 2016)
- Materials Data Curation System (February 2016)

NDS Labs technologies used:

- OpenStack GUI (required account setup)
- SSH terminal window (using public and private keys)

MGI Code Catalog



NIST Material Genome Initiative

MGI Code Catalog

NIST

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MGI Code Catalog

The MGI Code Catalog is an attempt to build a comprehensive list of available codes relevant to computational materials science and materials data analysis. It is build on the NIST developed Materials Data Curation System (<https://github.com/usnistgov/MDCS>).

The Materials Genome Initiative is fostering the acceleration of the discovery, design, development and deployment of new materials through the creation of a “Materials Innovation Infrastructure”. This infrastructure is comprised of computational tools, experimental tools, and digital data. In order to ensure the validity of computations, codes must be benchmarked and their quality assessed, which in turn requires knowledge of the currently available codes and methods.

The MGI Code Catalog is different from many of the other, similar, entities, in that it incorporates an extensive and extendible set of metadata, enabling fine-grained search. NIST is committed to maintaining this catalog, to ensure its accuracy and completeness, but the MGI Code Catalog cannot stay accurate and complete without community participation. If you’re aware of a code that should be listed here, we welcome your input.

To add new code to the MGI Code Catalog, [login](#) or [register](#) for an account.

Search the Catalog

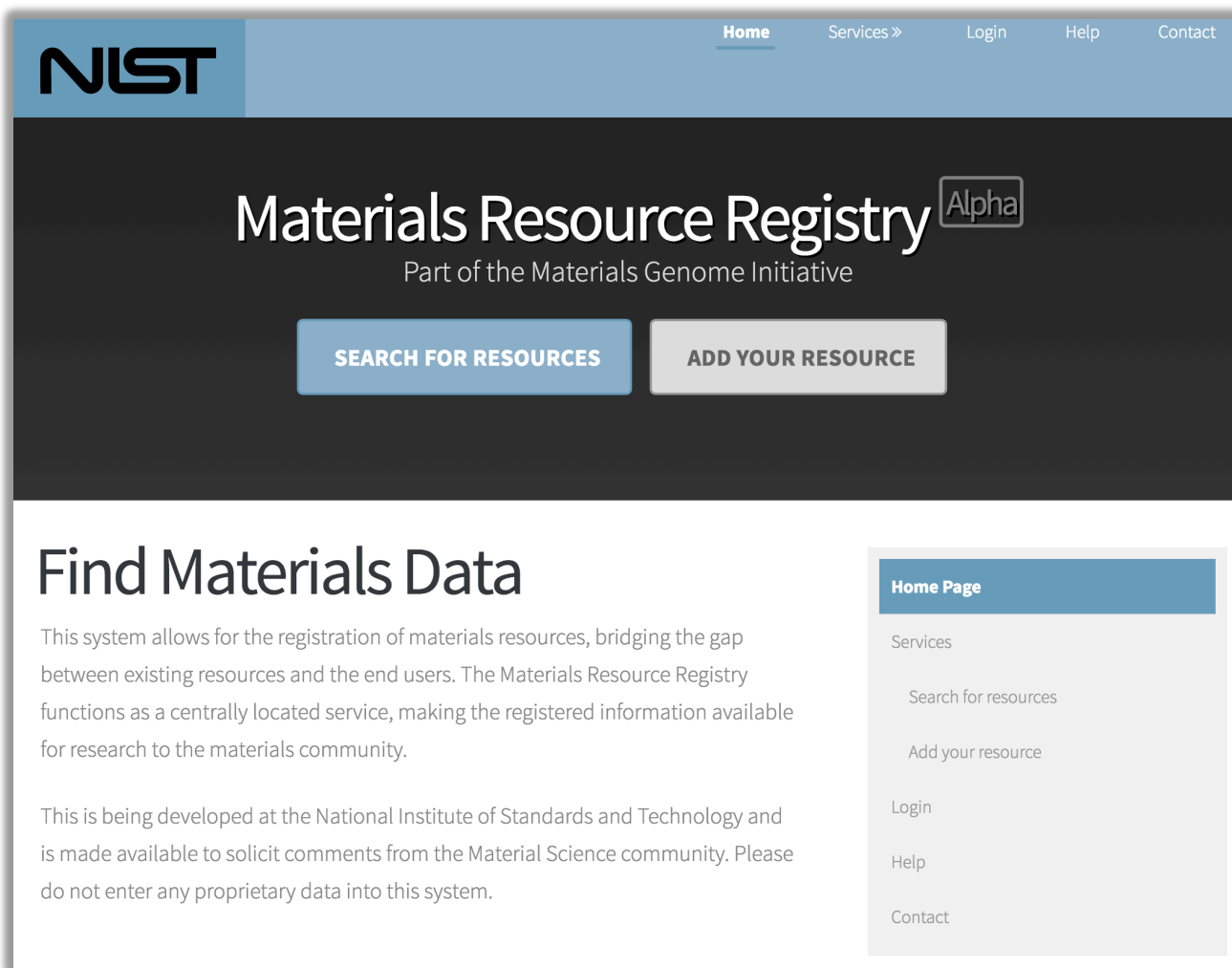
- [Explore records](#)

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Success Story #1 – <http://bit.ly/MGICodeCatalog>

NIST Materials Resource Registry



Success Story #2 – <http://bit.ly/MaterialsResourceRegistry>

Materials Data Curation System

Materials Data Curation System

Part of the Materials Genome Initiative

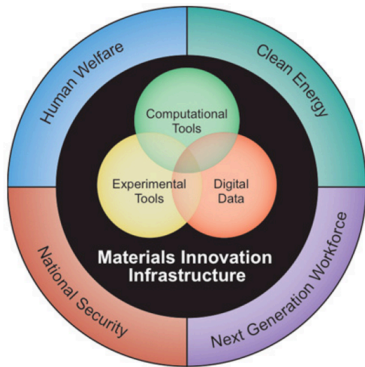
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Materials Data Curator

This system allows for the curation of Material Data in a repository using predefined templates.

This is being developed at the National Institute of Standards and Technology and is made available to solicit comments from the Material Science community. Please do not enter any proprietary data into this system.



The diagram illustrates the Materials Innovation Infrastructure. It features a central black circle labeled 'Materials Innovation Infrastructure'. Surrounding this center are four overlapping colored circles: 'Computational Tools' (green), 'Experimental Tools' (yellow), 'Digital Data' (orange), and 'Next Generation Workforce' (purple). These four circles are further enclosed by a larger ring divided into four segments: 'Human Welfare' (blue), 'Clean Energy' (teal), 'National Security' (red), and 'Next Generation Workforce' (purple).

Available Options

[All Options »](#)

Most Recent Templates

[Browse All »](#)

species-qs species.xsd.xml
TEM-Tutorial-Tamu workshop-TEM.xsd
TEM-Tut workshop-TEM.xsd

Success Story #3 – <http://bit.ly/MaterialsDataCurationSystem>

Current NDS Labs

Instantiate VM



SSH to VM



Deploy

The screenshot shows the OpenStack dashboard interface. On the left is a sidebar with navigation links: Project, Compute, Overview, Instances (highlighted in red), Volumes, Images, Access & Security, Network, Orchestration, and Identity. The main content area is titled 'Instances' and includes a search bar for 'Instance Name' and several action buttons: 'Launch Instance', 'Terminate Instances' (in red), and 'More Actions'. Below this is a table of instances.

<input type="checkbox"/>	Instance Name	Image Name	IP Address	Size	Key Pair	Status	Availability Zone	Task	Power State	Time since created	Actions
<input type="checkbox"/>	MGI Code Catalog v1.0	Ubuntu 14.04	192.168.100.7 Floating IPs: 141.142.209.106	r1.medium	MGI-cc2	Active	nova	None	Running	3 months, 2 weeks	Create Snapshot ▾
<input type="checkbox"/>	Materials Resource Registry vAlpha Chandler	Ubuntu 14.04	192.168.100.11 Floating IPs: 141.142.209.111	r1.medium	MMR	Active	nova	None	Running	3 months	Create Snapshot ▾
<input type="checkbox"/>	Materials Data Curation System v1.3	Ubuntu 14.04	192.168.100.13 Floating IPs: 141.142.209.110	r1.medium	MDCS	Active	nova	None	Running	1 month, 3 weeks	Create Snapshot ▾
<input type="checkbox"/>	Materials Resource Registry vAlpha Sandbox	Ubuntu 14.04	192.168.100.15 Floating IPs: 141.142.210.124	m1.medium	MMR	Active	nova	None	Running	1 month, 3 weeks	Create Snapshot ▾

Source: <https://nebula.ncsa.illinois.edu/dashboard/project/instances/>

Current NDS Labs

To add a new pilot to NDS Labs, we do the following:

1. Instantiate a VM using the OpenStack GUI
2. Specify security policy and associate a public floating IP
3. SSH into the new VM
4. Install the pilot software and Deploy

NDS Labs technologies used:

- ▣ OpenStack GUI (required account setup)
- ▣ SSH terminal window (using public and private keys)

Future NDS Labs (alpha)

The screenshot shows the NDS Labs web interface. At the top, the header includes the NDS Labs logo, the project name "Sharief", and user controls "Sharief" and "Sign Out". Below the header, the main content area is divided into a left sidebar and a main panel. The sidebar contains a "Find Services" search bar and a list of services: Clowder, Dataverse, iRODS iCAT, and Kibana (ELK), each with a "+" button. The main panel has tabs for "Stacks" and "Volumes". A large dashed box in the center of the main panel contains the text: "It looks like you haven't configured any stacks" and "Search and add a stack of services to see and manage it here". An "Auto Refresh" button is located in the top right of the main panel. At the bottom right, the footer displays version and timestamp information: "UI v1.0-alpha 2016-03-31 19:57" and "API v1.0-alpha 2016-04-01 11:51".

NIST Pilots
will go here

Future NDS Labs (alpha)

To add a new pilot to NDS Labs, we now do the following:

1. Find or create a Docker image (NIST pilot projects)
2. Create an NDS Labs service specification (via JSON service spec)
3. Add our specification to the service catalog (via ndslabsctl command)
4. Launch the service (view the NDS Labs GUI)

NDS Labs technologies used:

- ▣ Docker (<https://www.docker.com/>) and Docker Hub
- ▣ Kubernetes (<http://kubernetes.io/>)

Thank You – Questions?

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MGI Code Catalog

<http://bit.ly/MGICodeCatalog>

NIST Materials Resource Registry

<http://bit.ly/MaterialsResourceRegistry>

Materials Data Curation System

<http://bit.ly/MaterialsDataCurationSystem>

Presented at 5th National Data Service Consortium
Workshop in Chapel Hill, North Carolina.

Sharief Youssef (NIST)

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