Deployment of NIST Pilots on NDS Labs

Alden Dima, Chandler Becker, Phillippe Dessauw, Marcus Newrock, Raymond Plante, Pierre-François Rigodiat, Xavier Schmitt, Guillaume Sousa Amaral, Sharief Youssef

Information Systems Group – Mary Brady, Group Leader

Office of Data and Informatics – Robert Hanisch, Director

Information Technology and Material Measurement Laboratories

National Institute of Standards and Technology (NIST)
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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

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 extensible 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.
Find Materials Data

This system allows for the registration of materials resources, bridging the gap between existing resources and the end users. The Materials Resource Registry functions as a centrally located service, making the registered information available for research to the materials community.

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.
Materials Data Curation System

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.

Available Options

Most Recent Templates

Current NDS Labs

- Instantiate VM
- SSH to VM
- Deploy

Source: https://nebula.ncsa.illinois.edu/dashboard/project/instances/
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)
It looks like you haven't configured any stacks
Search and add a stack of services to see and manage it here

NIST Pilots will go here

Source: 5th National Data Service Consortium Workshop Tutorials
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/](https://www.docker.com/)) and Docker Hub
- Kubernetes ([http://kubernetes.io/](http://kubernetes.io/))
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MGI Code Catalog
NIST Materials Resource Registry
Materials Data Curation System

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

Sharief Youssef (NIST)
Email: sharief.youssef@nist.gov