



## NDS Labs Workbench + DataDNS

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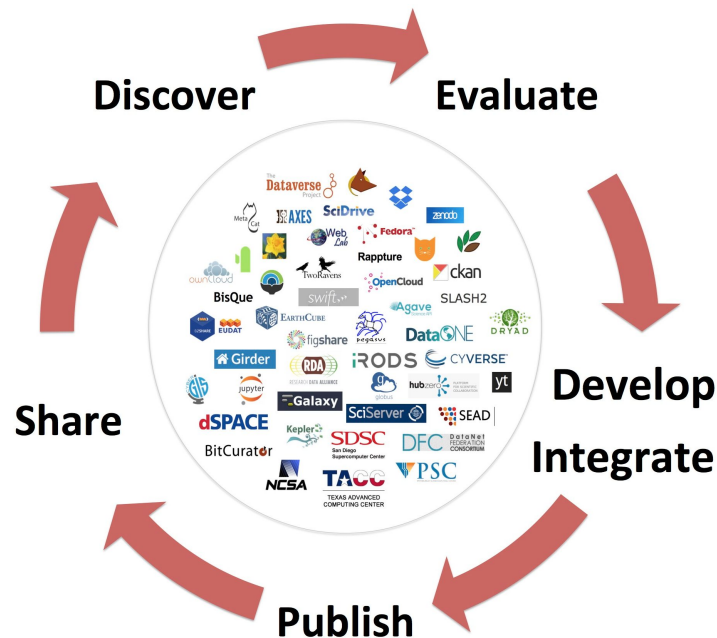
Container Analysis Environments Workshop  
August 14, 2017



# NDS Labs Workbench (beta)

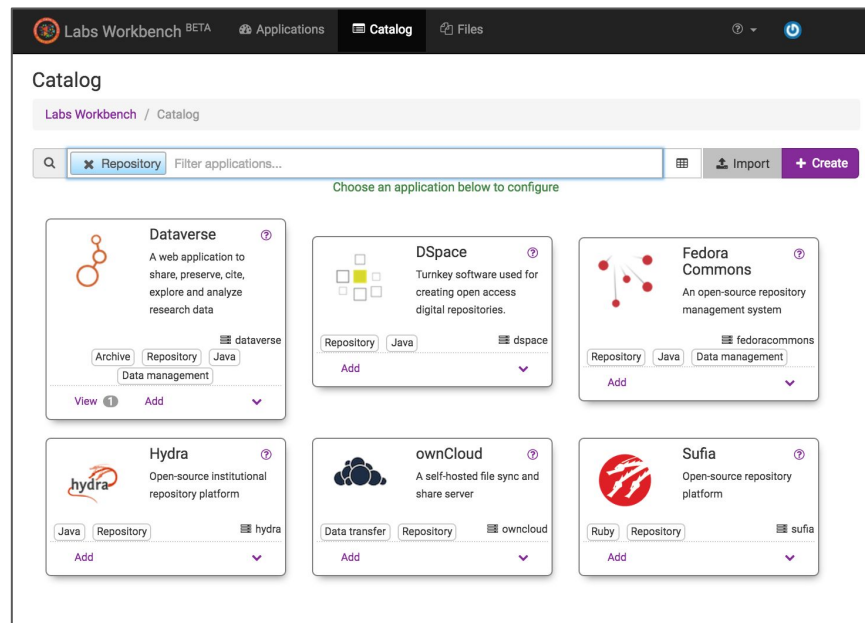
<https://www.workbench.nationaldataservice.org>

- NDSC initiative started in January 2016
- Community-driven platform to share, discover, evaluate, develop, and test research data management and analysis tools
- Open platform -- community members recommend and/or contribute tools



# NDS Labs Workbench

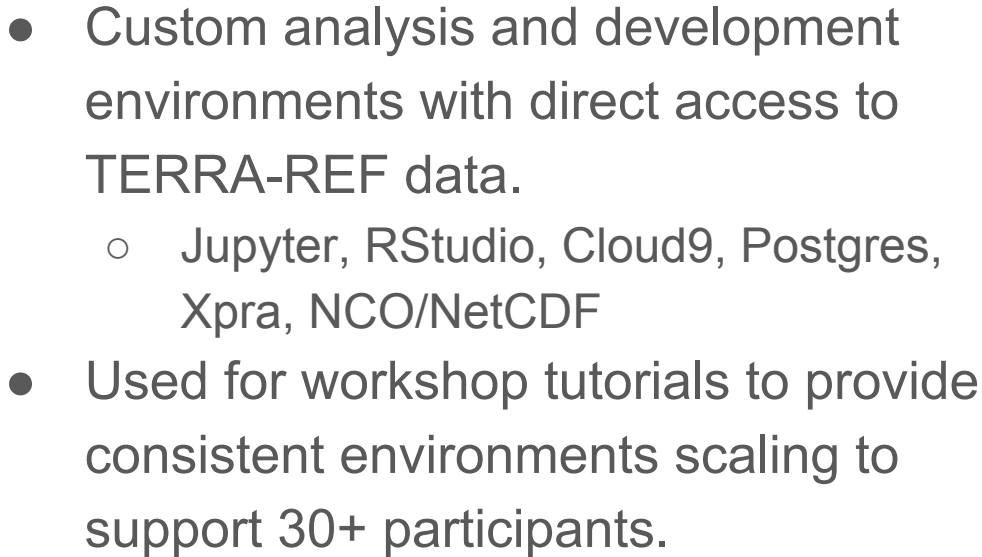
- Scalable platform (Kubernetes/OpenStack)
- Web-based, turn-key system for the deployment of data tools
- Includes catalog of community-contributed tools
- A personal test environment or sandbox
- Personal catalogs
- Console access to all applications



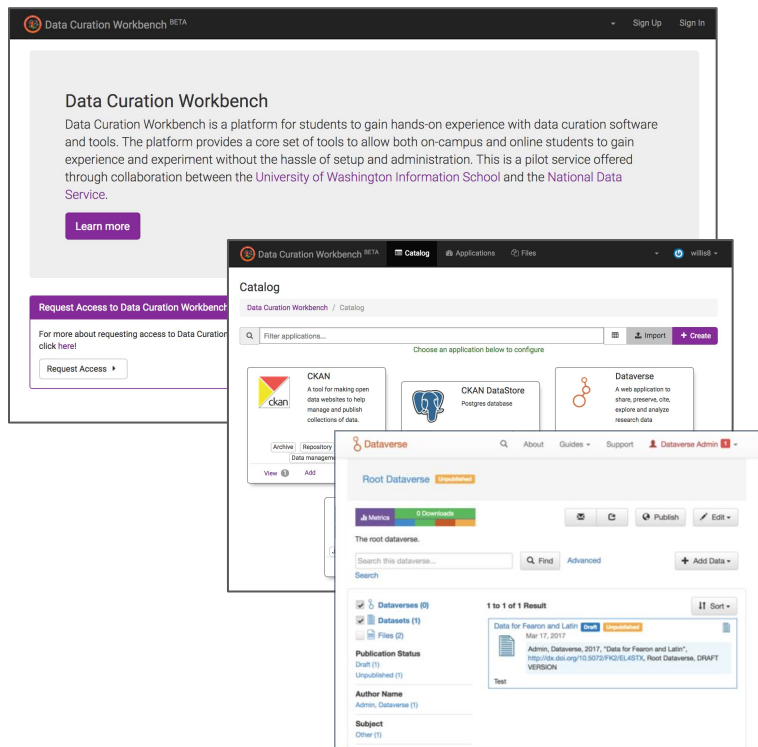
## Driving user stories

1. A **developer** is assigned to a new data-related project and tasked with 1) learning, 2) evaluating or 3) extending data-related services.
2. An **instructor** wants to incorporate hands-on experience data management or analysis tools into a workshop or course.
3. **Students** or **workshop** participants need access to specialized software environments and real datasets (over hotel wifi, on tablets).
4. **Researchers** (and developers) associated with the same project need ongoing **remote access to data and software** required to access it.

## Use case: TERRA-REF Analysis Workbench

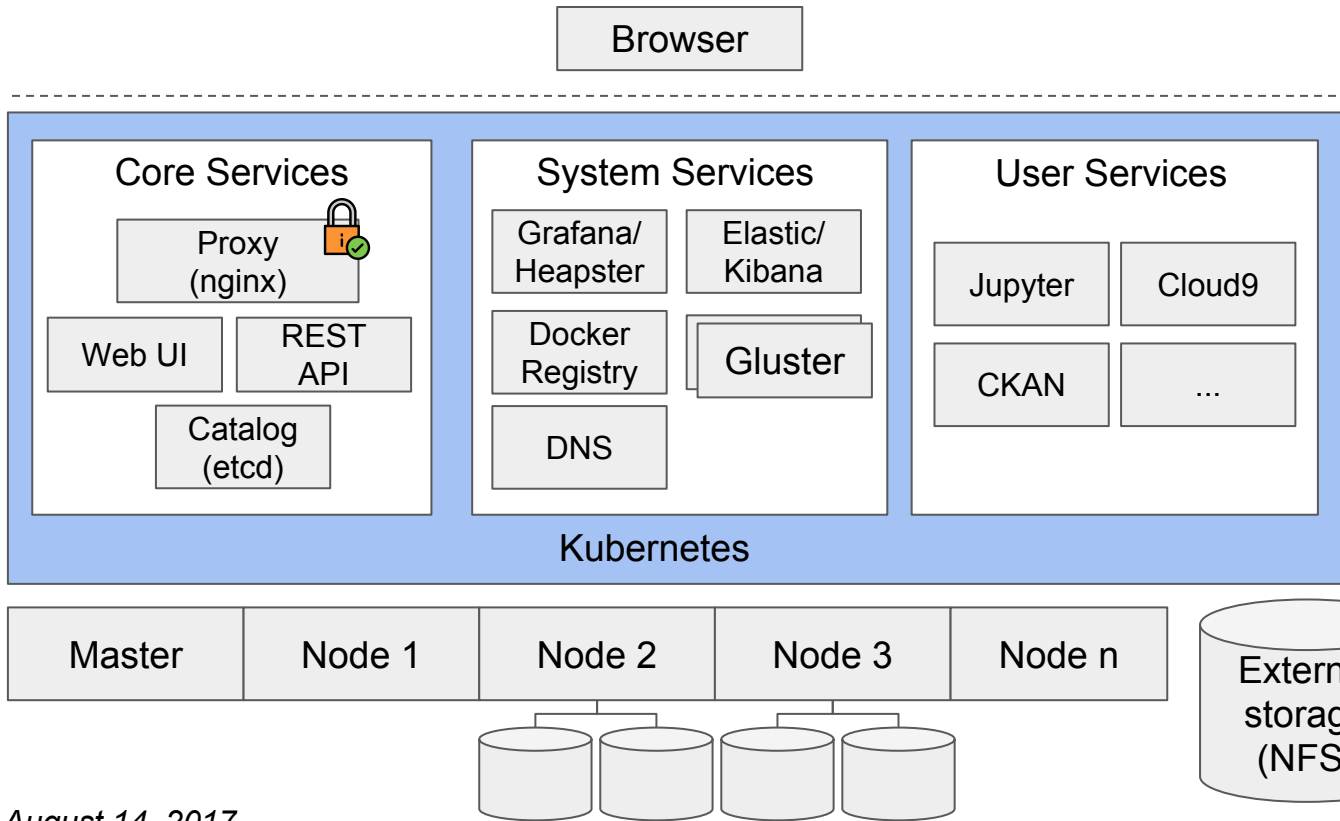


# Use case: Data Curation Education Workbench

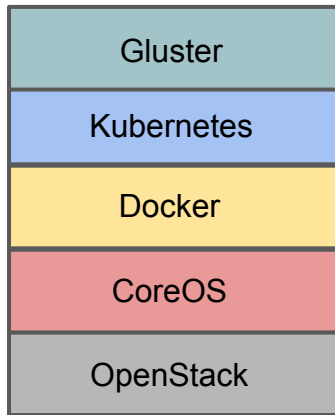


- Ongoing pilot project led by University of Washington iSchool
- Customized instance of Labs Workbench hosted on SDSC Cloud
- Sandbox for students to get hands-on experience with data curation systems and tools including CKAN and Dataverse.

# Labs Workbench Architecture Overview



## Technologies:



# Why Docker and Kubernetes?

- Why Docker?
  - Installing/configuring many of these applications is not easy
  - Simplifies dependency management
  - Fast
  - Opportunity for preservation
- Why Kubernetes?
  - Scalable, reliable
  - Runs everywhere (OpenStack, AWS, GCE, Azure)
  - Resource constraints, scheduling, batch/job support
  - Many "free" services (NGINX proxy, LMA, cluster local DNS)



## Other features

- Other features
  - Multiple-service applications (web + database + etc)
  - X-Windows application support via NoVNC/Xpra
  - Configurable service timeouts
  - Customizable UI
  - Account approval

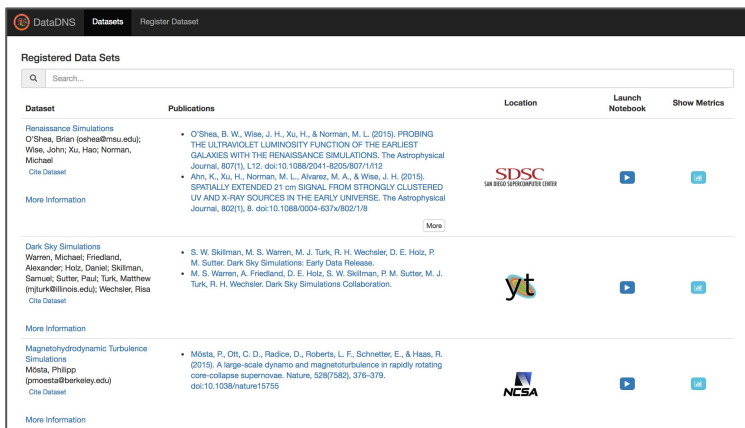
# Challenges










- Storage
  - Shared storage -- particularly performance
  - Permissions, ownership
- Getting contributors to create their own images
- Single sign-on
- Versioning/management of images/dependencies
- Requires wildcard DNS/TLS
- Kubernetes -- complex and fast moving
  - Not easy to install on OpenStack

## On the horizon:

- Single sign-on (CILogon)
- Integration with cloud/HPC systems
  - Head node replacement
  - Shared authentication, filesystems
- Simplified installation (simplicity + scalability)
- Support commercial cloud environments

# DataDNS: Discovery, access, and in-place analysis for large scale data

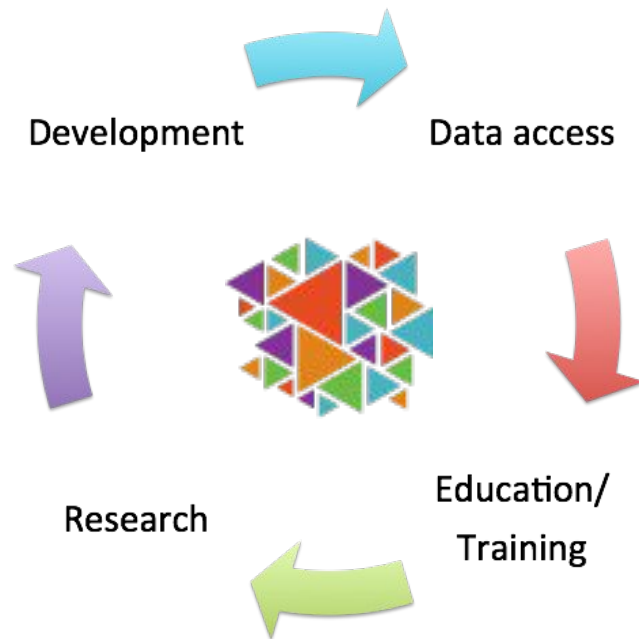


Dataset	Publications	Location	Launch Notebook	Show Metrics
<b>Renaissance Simulations</b> O'Shea, Brian (bpoheal@msu.edu), Wise, John, Xu, Hao, Norman, Michael <a href="#">Cite Dataset</a>	<ul style="list-style-type: none"> <li>O'Shea, B. W., Wise, J. H., Xu, H., &amp; Norman, M. L. (2015). PROBING THE ULTRAVIOLET LUMINOSITY FUNCTION OF THE EARLIEST GALAXIES WITH THE RENAISSANCE SIMULATIONS. <i>The Astrophysical Journal</i>, 807(1), L12. doi:10.1088/2041-8205/807/1/L12</li> <li>Ahn, K., Xu, H., Norman, M. L., Alvarez, M. A., &amp; Wise, J. H. (2015). SPATIALLY EXTENDED 21 cm SIGNAL FROM STRONGLY CLUSTERED UV AND X-RAY SOURCES IN THE EARLY UNIVERSE. <i>The Astrophysical Journal</i>, 802(1), 8. doi:10.1088/0004-637x/802/1/8</li> </ul> <a href="#">More Information</a>			
<b>Dark Sky Simulations</b> Warren, Michael, Friedland, Alexander, Holz, Daniel, Skillman, Samuel, Sutter, Paul, Turk, Matthew (mturk@illinois.edu), Wechsler, Risa <a href="#">Cite Dataset</a>	<ul style="list-style-type: none"> <li>S. W. Skillman, M. S. Warren, M. J. Turk, R. H. Wechsler, D. E. Holz, P. M. Sutter, Dark Sky Simulations: Early Data Release.</li> <li>M. S. Warren, A. Friedland, D. E. Holz, S. W. Skillman, P. M. Sutter, M. J. Turk, R. H. Wechsler. Dark Sky Simulations Collaboration.</li> </ul> <a href="#">More Information</a>			
<b>Magnetohydrodynamic Turbulence Simulations</b> Mösta, Philipp (pmosta@berkeley.edu) <a href="#">Cite Dataset</a>	<ul style="list-style-type: none"> <li>Mösta, P., Ott, C. D., Radice, D., Roberts, L. F., Schnetter, E., &amp; Haas, R. (2015). A large-scale dynamo and magnetoturbulence in rapidly rotating core-collapse supernovae. <i>Nature</i>, 529(7582), 378-379. doi:10.1038/nature15755</li> </ul> <a href="#">More Information</a>			

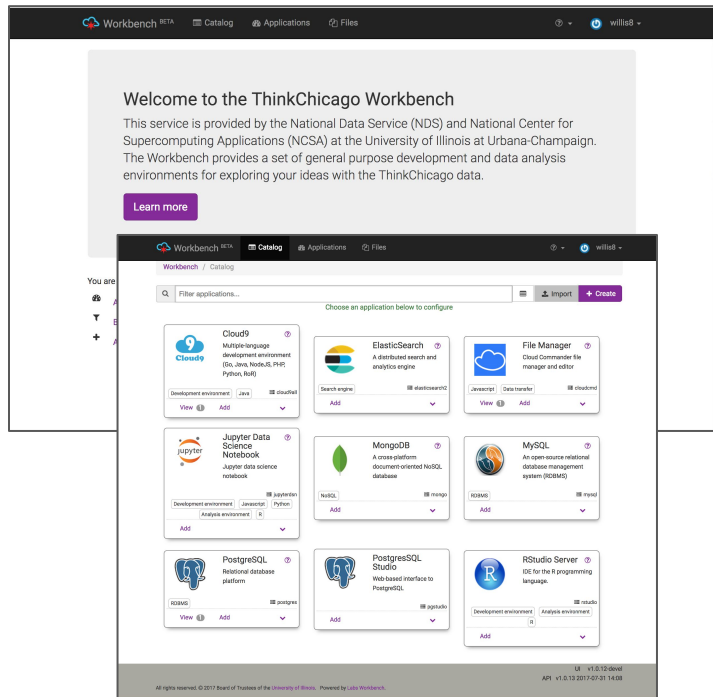
- Emerging vision from NDSC
- Data analysis and compute discovery engine.
- Connecting services that provide in-place access to data analysis environments.
- Defines common interface for heterogeneous environments.

# Labs Workbench Platform

- Software packaged as containers
- Enables rapid deployment on scalable infrastructure
- To facilitate:
  - In-place data access
  - Research/development
  - Education/training



# Use case: ThinkChicago Tech Challenge



- Hackathon supported by University of Illinois System and City of Chicago.
- 200 students (in teams of 10) present ideas centered around government data.
- Each team had access to common development tools and data via customized Labs Workbench.

