

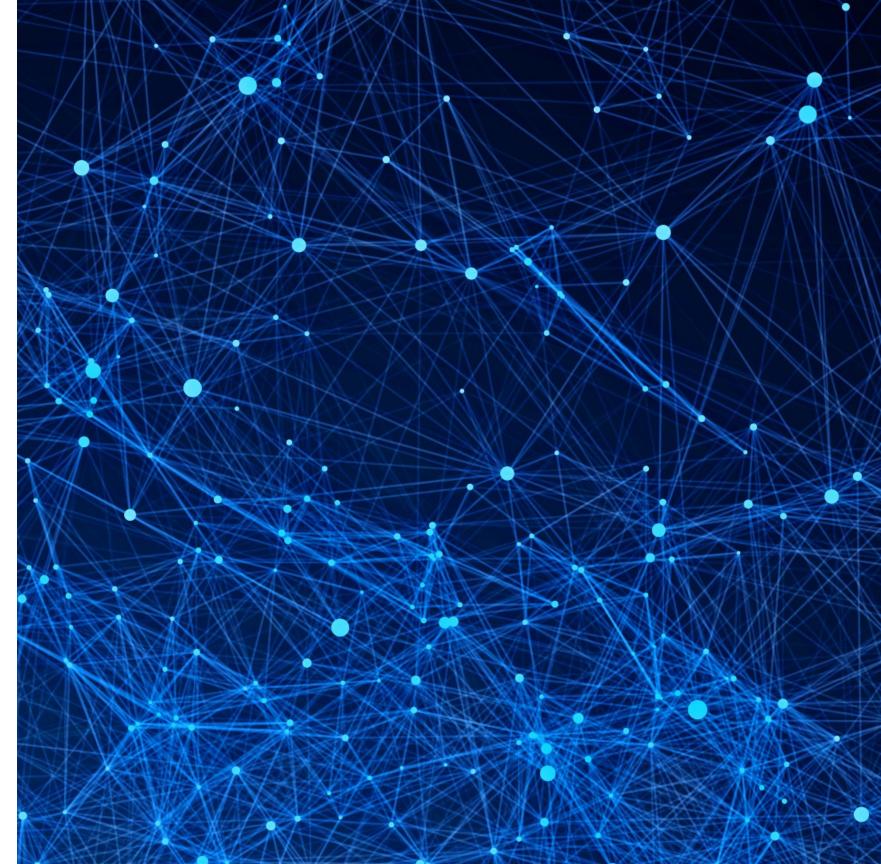


FY23 Updates to the MSD-LIVE Data and Computational Platform

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The Vision for MSD-LIVE







Visit us at https://msdlive.org



Data & Code Repository

Discover and share curated MSD datasets, codes, and workflows.



Project Services

Create and manage project teams and their collaborative tools



Computational Resources

Use Jupyter Notebooks to analyze or visualize data stored in MSD-LIVE.



Get Started

Learn how to start using MSD-LIVE to manage your data.

- A cloud-based data management system and advanced computing platform
- Will enable researchers to document and archive their data, run their models and analysis tools, and share data, software, and multi-model workflows
- A cornerstone capability of the MSD Community of Practice

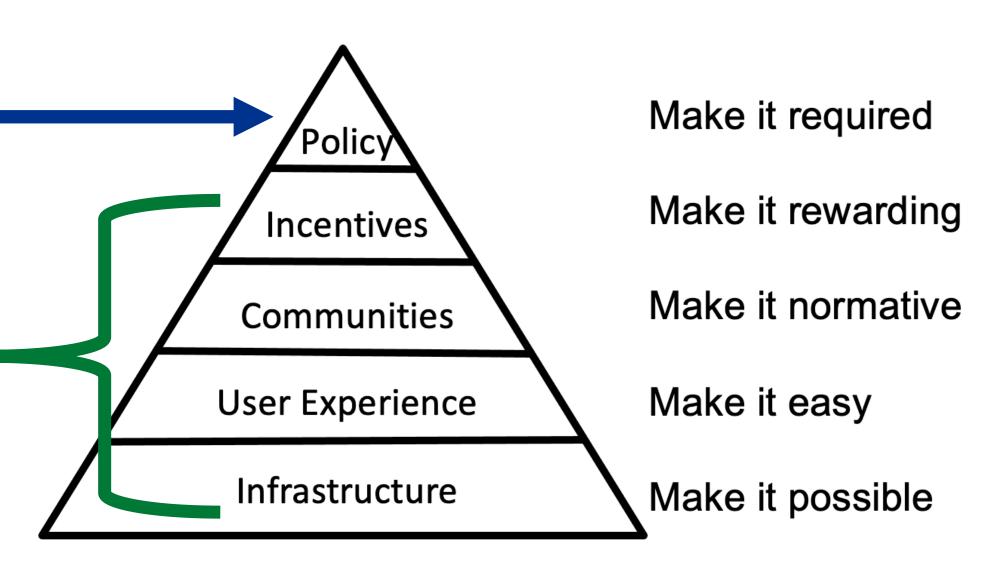


Facilitating Open MSD Science



Journals largely skipped to this end of the pyramid...

MSD-LIVE is about tackling these foundational elements of the pyramid...



Conceptual diagram from Brian Nosek of the University of Virginia and the Center for Open Science



Top-10 Most Pressing Use Cases MSD



Use Case	Name	Description	
1.1	Find Data	Quickly and easily find datasets produced by other users and projects	
1.2	Archive Data	Permanently archive small (<250 MB), medium (250 MB - 50 GB), and large (50 GB to 20 TB) final-form datasets and generate data Digital Object Identifiers (DOIs) in order to meet journal requirements for data sharing	
1.3	Version Control		
1.4	Training	Train new team members on MSD projects to effectively manage data and code and capture the institutional knowledge of members that leave a project	
1.5	Control Access	Create and manage teams that cross institutions in order to quickly and easily grant access to data and code without having to obtain multiple sets of institutional credentials	
2.1	Share Data	Share working datasets across multiple institutions collaborating on a project in real-time	
2.2	Analyze Data	Create, run, and share Jupyter notebooks to analyze or visualize datasets in MSD-LIVE	
2.3	Multi-Model Create, execute, document, and publish multi-model workflows where component models run on computational resources at different institutions		
2.4	Virtually assemble data lakes and execute ML/AI algorithms on large pools of data that may be physically located in different places		
2.5	Move Code to the Data	Easily deploy models to run on new computational resources and make it easy for users to bring their code to the data when transferring data is infeasible	



= in v1 release

Milestones and Capabilities



Core Capabilities	Use Cases
	Find Data
	Archive Data
Data Repository	Version Control
	Training
	Control Access
	Share Data
	Analyze Data
Advanced Computing	Multi-Model Workflows
	ML/AI
	Move Code to the Data

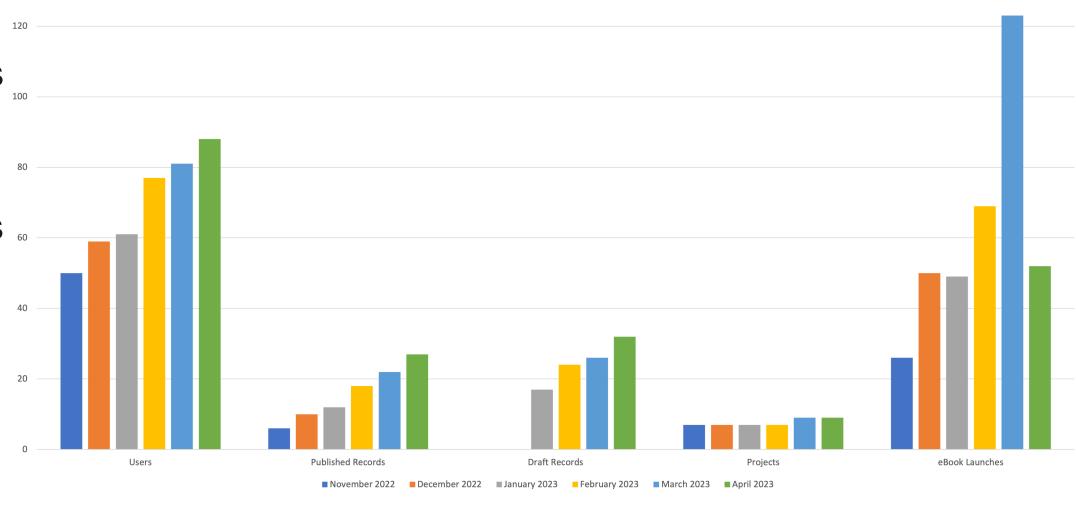
- Feb-22: Beta version of the data repository released for testing by our stakeholder group.
- Jun-22: The "Addressing Uncertainty in MultiSector Dynamics Research" eBook was migrated to MSD-LIVE. The eBook contains on-demand, interactive tutorials for common UC/UQ workflows.
- Aug-22: v1 of MSD-LIVE released to the MSD research community.
- Jun-23: v2 release includes better ways to move large data in and out of MSD-LIVE.
- Jun-23: Used to facilitate training sessions during the GCAM annual meeting. Participants can run the hector, stitches, and xanthos models in real-time on the AWS cloud.



Usage Statistics



- 9 registered projects
- 88 registered users
- 27 published datasets and 32 open draft datasets
- 186+ Tb of total data
- 52 usages of the MSD UC eBook
 Jupyter notebooks in the last 30 days





v2 Released Today!



- In v2: Data repository updates
 - Dedicated storage buckets by project
 - Ability to upload nested folder hierarchies instead of zip files
 - Upload via the command-line in addition to the web portal
- Coming in v3: Compute services
 - Ability to create a Jupyter notebook to analyze or visualize data
 - Ability to manage collection of Jupyter notebooks (e.g., GitHub integration)
 - Allow notebooks to be directly connected to MSD-LIVE datasets
 - Automated support for training and demonstrations using Jupyter notebooks
- Coming in v3: Deployment environment
 - Protocols in place for tracking cost and usage by project

Green = Completed; Orange = In Progress; Red = Not Started



New Command-Line Interface



Use the MSD-LIVE CLI

- Python package that installs directly from pip
- Simple one-line commands for uploading and downloading large datasets
- Utilizes AWS-native file transfer protocols on the backend
- Fast, easy to use, and allows for easy recovery from interrupted transfers

◆ Install The CLI

To install the CLI, run this command from your computer terminal:

pip install https://github.com/MSD-LIVE/msdlive-cli-distro/raw/dev/dist/msdlive_cli0.3.0-py3-none-any.whl

c

Note

- The MSD-LIVE CLI requires Python 3.8 or higher. If you get a "command not found" error when trying to run pip, then you must install Python or use conda (see below).
- If you encounter dependency conflicts when installing, we recommend using a Python virtual environment such as venv or conda.

Authenticate

Download Files

Replace "MY_LOCAL_DIR" with the path to the directory where the files should be saved.

msdlive download --dataset-id y24zr-ntq50 --output-dir MY_LOCAL_DIR



Upload Files

Replace "MY_LOCAL_DIR" with the path to the directory containing your files.

msdlive upload --dataset-id y24zr-ntq50 --src-dir MY_LOCAL_DIR



Note

• If you are using a Python virtual environment, make sure to activate it before running any CLI commands from your terminal!

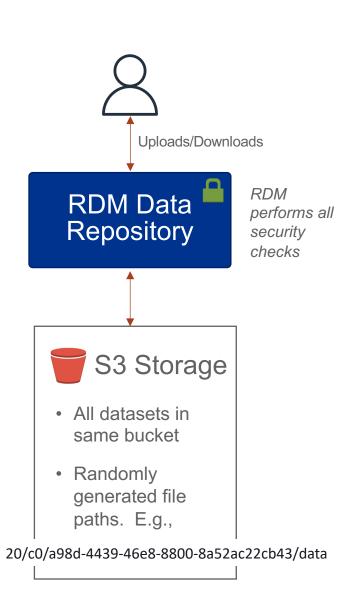


Changes to MSD-LIVE File Storage



Before

- Uploads go through RDM = 2 hops!
- Network interruptions not recoverable
- Folders not supported
- Not accessible outside RDM
- Unreadable file names



After

- Uploads direct to S3
- Uploads can recover from network interruptions
- Folder
 hierarchy and
 file names
 preserved
- Directly
 accessible by
 users and other
 AWS compute
 resources

