

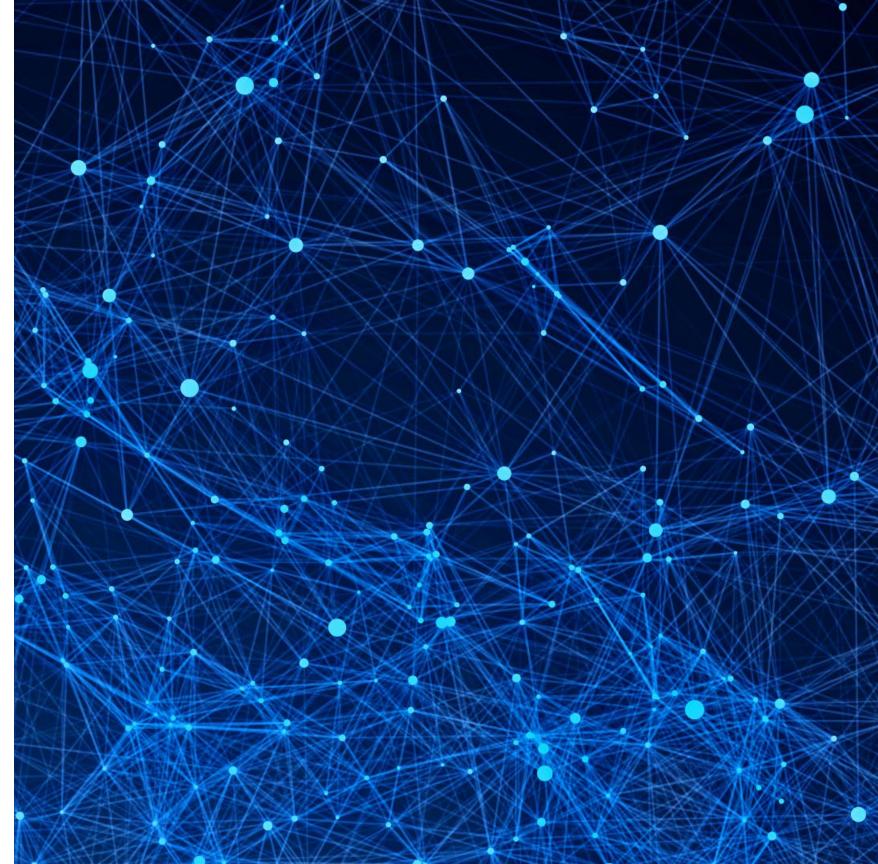


The MSD-LIVE Data and Computational Platform

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PNNL is operated by Battelle for the U.S. Department of Energy

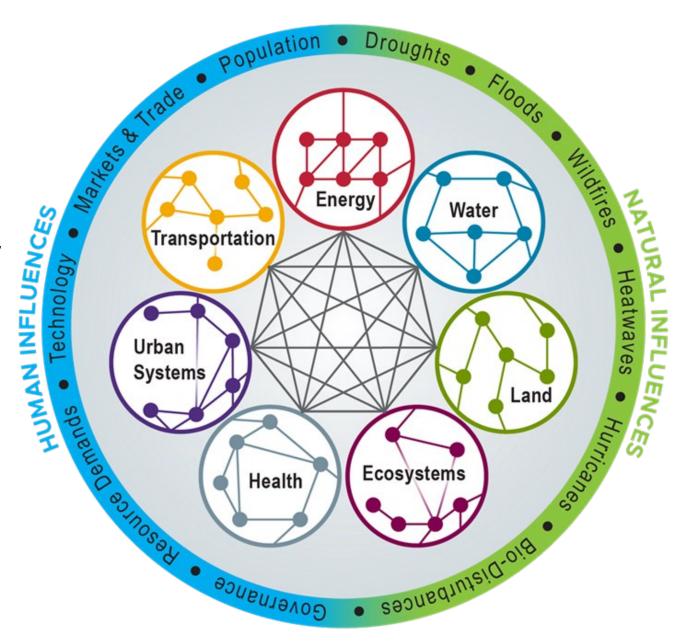




MultiSector Dynamics (MSD) Overview



- Multisector dynamics refers to the complex interactions and interdependencies that exist among different sectors of human and natural systems. It involves understanding how changes and developments in one sector can influence and impact other sectors.
- The importance of studying multisector dynamics lies in the recognition that no sector operates in isolation. Economic, social, and environmental systems are interconnected, and changes in one sector can have cascading effects across multiple sectors



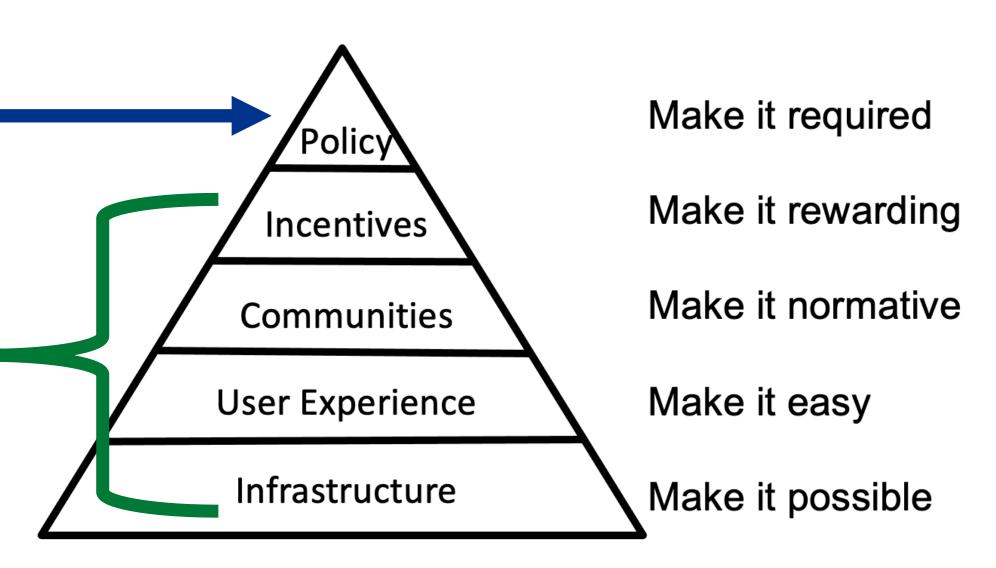


Facilitating Open Science with MSD-LIVE



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

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



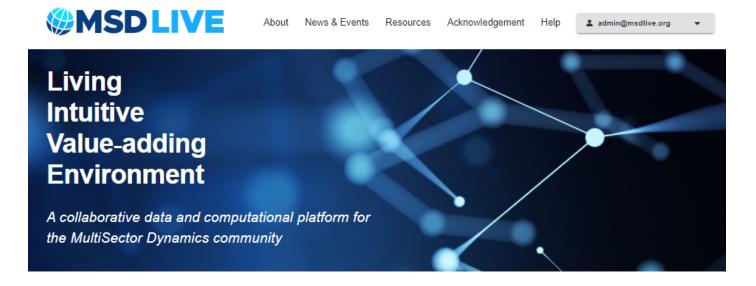
Conceptual diagram from Brian Nosek of the University of Virginia and the Center for Open Science



The Vision for MSD-LIVE



- Cloud-based flexible and scalable data management system and advanced computing platform
- Custom-built to meet the needs of the MSD program area within DOE's Office of Science
- Intuitive user experience at scale:
 - Archive and share data
 - Share software and multi-model workflows
 - Run models and analysis tools





Data & Code Repository

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



Computational Resources

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



Project Services

Create and manage project teams and their collaborative tools and resources.



Get Started

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

MSD-LIVE is being developed with support from the MultiSector Dynamics program area within the Earth and Environmental Systems Modeling program of the U.S. Department of Energy's Office of Science.





Why Not Use an Existing Solution?



Common issues with existing scientific data management systems:

- Not tailored to the MSD users (e.g., generic metadata)
- Poor performance and reliability when uploading/downloading large datasets
- Lack direct access to data for compute platform
- Folder hierarchies not supported
- Bad user experience: new users struggle to setup and use the system



The MSD-LIVE Approach

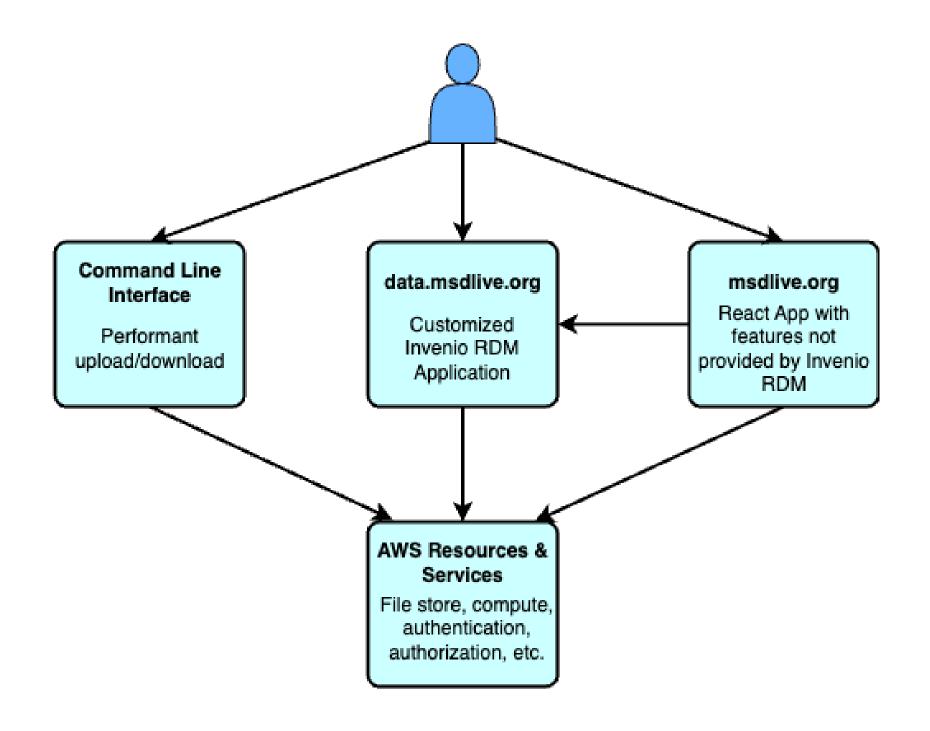


- Start with an open-source solution (Invenio RDM)
- Customize and extend it to achieve our goals
 - Customize metadata schema
 - Integrate with OSTI to mint DOIs
 - Add projects
 - Customize UI for seamless user experience
- Build everything on the cloud (AWS)
- Provide direct access to the data from Jupyter Notebook containers running in AWS
- Use AWS CloudFormation and AWS Cloud Development Kit to create version controlled and reusable infrastructure



High Level Architecture



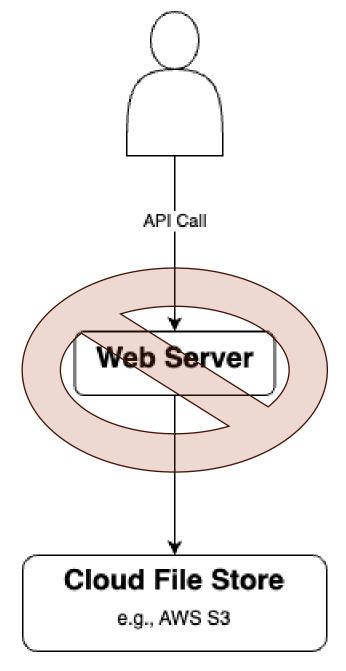




Direct Data Access: Why?



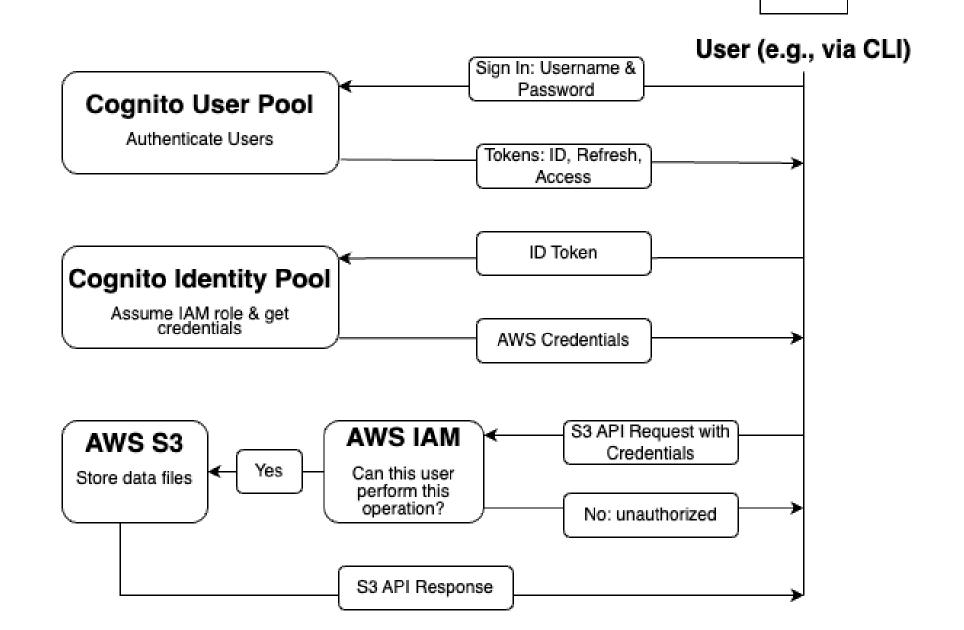
- Direct access: data and requests do NOT go through an intermediary web server
- Jupyter Notebooks can access data on the cloud in a secure way (i.e., with project-based access control)
- Allows us to use AWS open-source libraries on the client (e.g., the CLI and in the browser)
 - We don't reinvent the wheel
 - Code is well tested and performant





Direct Data Access: How it Works MSD







Demo Video



• Demo: <u>Using MSD-LIVE's CLI to upload files</u>



Current Notebooks



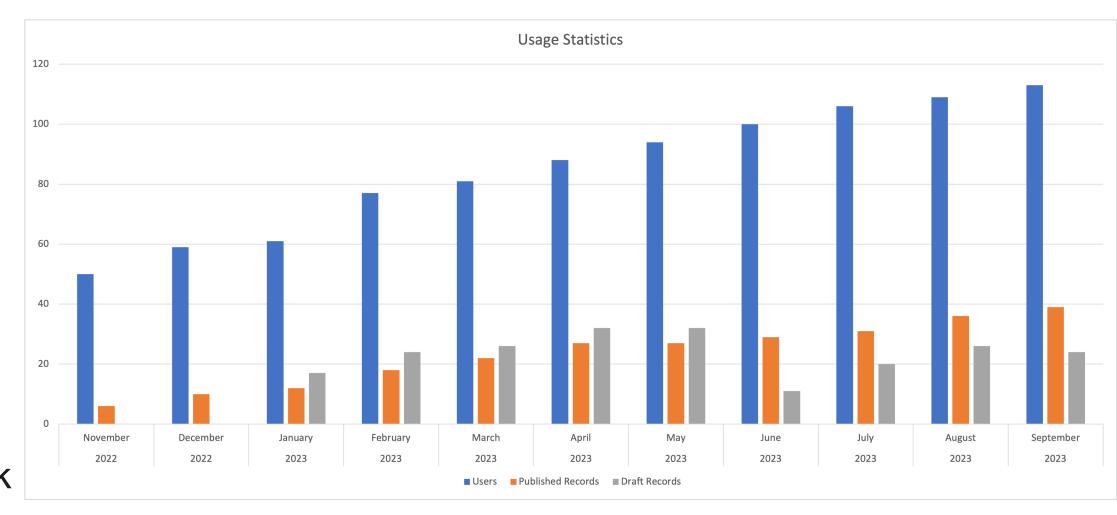
- Interactive model training notebooks:
 - > IM3 Uncertainty Characterization eBook: https://uc-ebook.org/
 - > GCIMS Xanthos: https://xanthos.msdlive.org
 - GCIMS Hector: https://hector.msdlive.org
 - > GCIMS GCAM Wrapper: https://gcamwrapper.msdlive.org
 - > GCIMS Stitches: https://stitches.msdlive.org
 - > IM3 StateModify: https://statemodify.msdlive.org
- Data dashboard:
 - PCHES https://lafferty-sriver-2023-downscaling-uncertainty.msdlive.org/user-redirect/lab/tree/dashboard.ipynb



Usage Statistics



- 9 projects
- 113 users from
 15 states and 4
 countries
- 39 published datasets and 24 open draft datasets
- 187+ Tb of data
- 518 uses of Jupyter notebook feature last month





Thank you!



Questions?