National Aeronautics and Space Administration

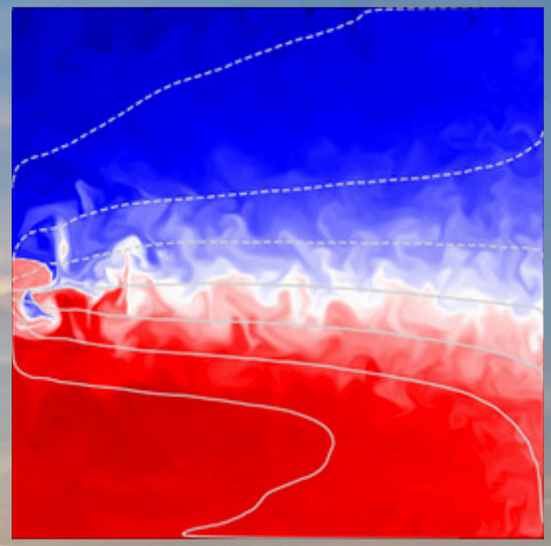
Transforming to Open Science: perspectives on how to best support open science

Paige E. Martin
Program Scientist
NASA Chief Science Data Office

MY BACKGROUND

PHYSICAL OCEANOGRAPHY

PhD @ University of Michigan

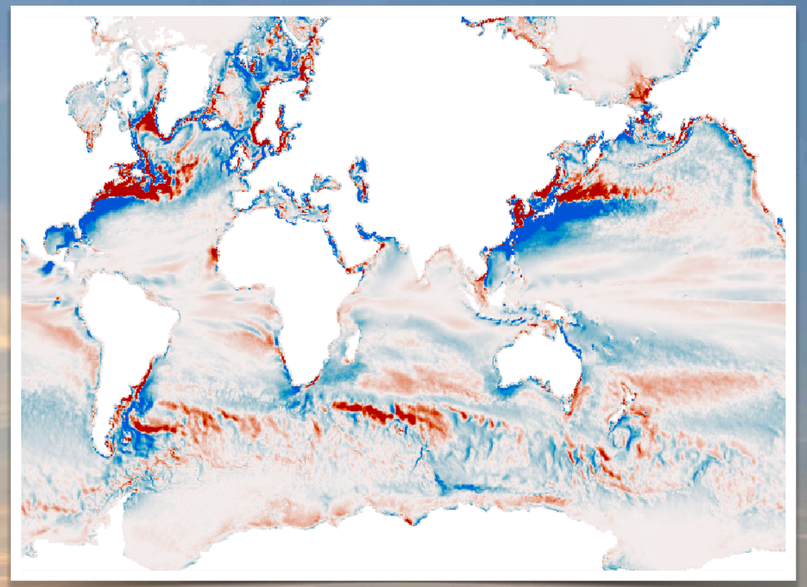


Energy budgets and temperature variance in idealized model

MY BACKGROUND

CLIMATE DATA SCIENCE

Postdoc @ Lamont Doherty
Earth Observatory



Air-sea interaction in CESM

CURRENTLY

NASA'S CHIEF SCIENCE DATA OFFICE

Program Scientist

NASA's Transform to Open Science (TOPS) & Open Source Science Initiative

A community for big data geoscience

WHAT IS PANGEO?

- Community obsessed with efficient data processing.

  Founded in 2016. Scientists and software developers coming together. http://pangeo.io/
  Weekly meeting / seminar. Discourse Forum. Annual meeting. Workshops at AGU / AMS / etc.

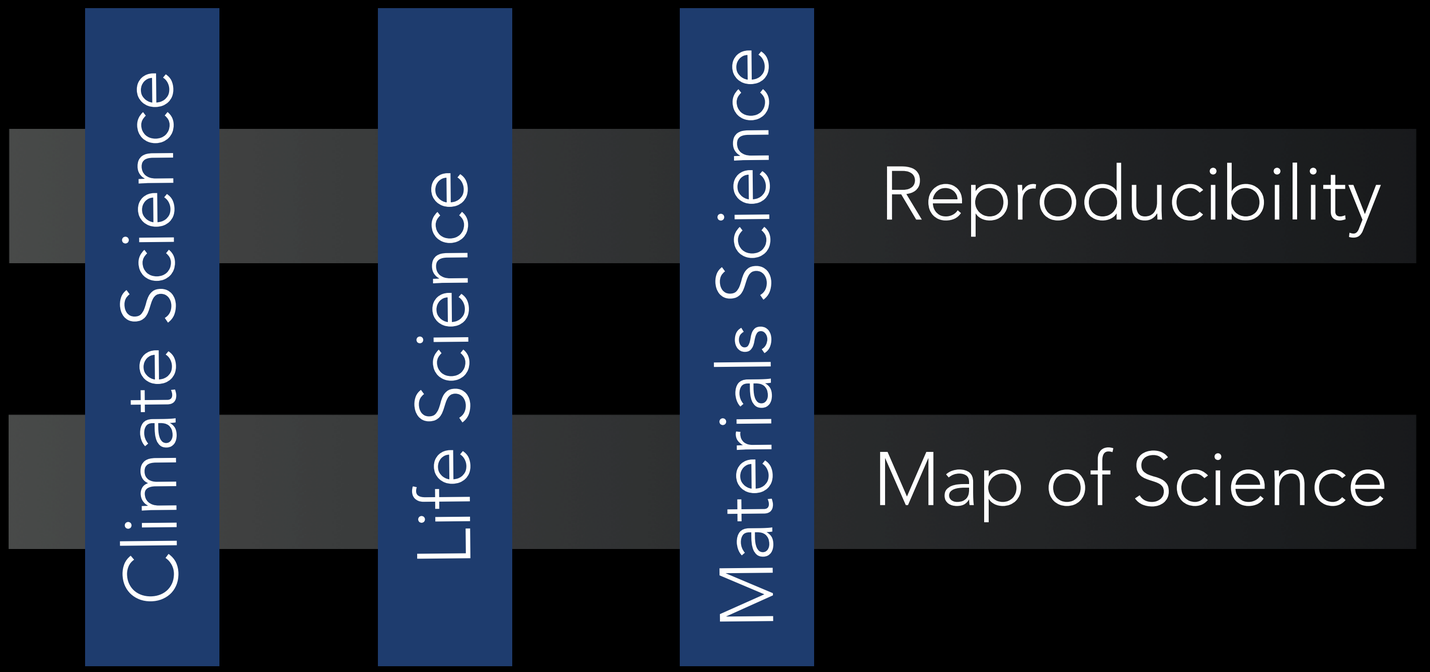
- Interoperable Software

  Foundation in Scientific Python: Jupyter, Xarray, Dask, Zarr. Broad ecosystem of interoperable packages for analysis, visualization, and machine learning.

- Data and Computing Infrastructure

  Deployment recipes for cloud and HPC. Open, public, cloud-based JupyterHubs and Binders for Data-proximate computing. PB of analysis-ready, cloud-optimized data stored in public cloud (GCS, AWS) and OpenStorageNetwork.

Open Source .Science



A community that brings together scientific users and software engineers to accelerate science

NUMFOCUS
OPEN CODE = BETTER SCIENCE

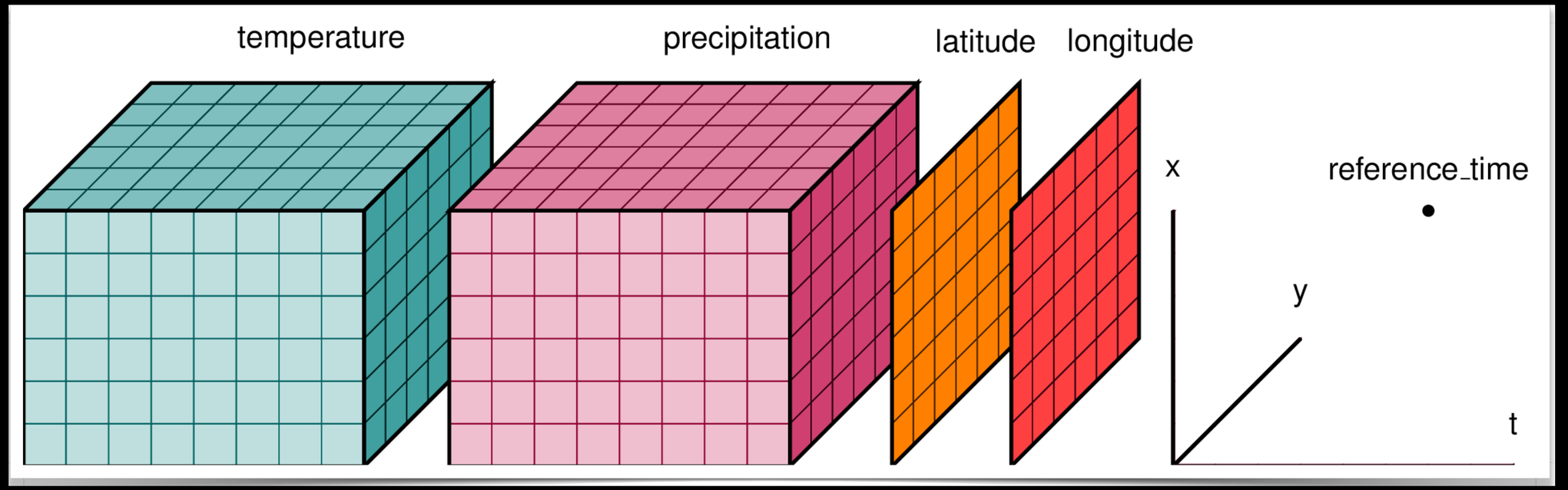
Pathways that guided me to open science

1. **<u>Accessibility:</u>** I lost access to Matlab 😢

Pathways that guided me to open science

1. **Accessibility:** I lost access to Matlab 😢
2. **Scalability:** open source software allowed for handling of my large, complex datasets 🤸

SCALABILITY



$$0 = 2\int\int\Bigg(\underbrace{-\mathrm{Re}\left[\widehat{{}^{o}T_m}^{*}\left(\widehat{{}^{o}u_m\,{}^{o}T_m}\right)_x\right]-\mathrm{Re}\left[\widehat{{}^{o}T_m}^{*}\left(\widehat{{}^{o}v_m\,{}^{o}T_m}\right)_y\right]}_{\text{horizontal advection}}+\underbrace{\frac{1}{{}^{o}H_m}\mathrm{Re}\left[\widehat{{}^{o}T_m}^{*}\,\widehat{{}^{o}w_{ek}\,{}^{o}T_m}\right]}_{\text{vertical advection}}+\overbrace{\frac{1}{{}^{o}\rho\,{}^{o}C_p\,{}^{o}H_m}\mathrm{Re}\left[\widehat{{}^{o}T_m}^{*}\widehat{F_m^{e+}}\right]}^{\text{entrainment heat flux}}-\overbrace{\frac{1}{{}^{o}\rho\,{}^{o}C_p\,{}^{o}H_m}\mathrm{Re}\left[\widehat{{}^{o}T_m}^{*}\widehat{F_\lambda}\right]}^{\text{sensible/latent heat flux}}-\overbrace{\frac{1}{{}^{o}\rho\,{}^{o}C_p\,{}^{o}H_m}\mathrm{Re}\left[\widehat{{}^{o}T_m}^{*}\left(\widehat{F_0^{\uparrow}+F_m^{\downarrow}}\right)\right]}^{\text{radiative heat flux}}$$

$$\underbrace{+\mathrm{Re}\left[\widehat{{}^{o}T_m}^{*}\,{}^{o}K_2\nabla_H^2\,\widehat{{}^{o}T_m}\right]-\mathrm{Re}\left[\widehat{{}^{o}T_m}^{*}\,{}^{o}K_4\nabla_H^4\,\widehat{{}^{o}T_m}\right]}_{\text{diffusion}}\Bigg)dxdy,$$

Pathways that guided me to open science

1. **Accessibility:** I lost access to Matlab 😢
2. **Scalability:** open source software allowed for handling of my large, complex datasets 🤸
3. **Inclusion:** open source (and free) software removed barriers to doing science 🥳

Mumin Olatunji Oladipo

Communication Physics, Nigeria
PhD Student (University of Ilorin)
Assistant Lecturer (KolaDaisi University, Ibadan)
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COASTAL OCEAN ENVIRONMENT SUMMER SCHOOL IN GHANA

coessing.org

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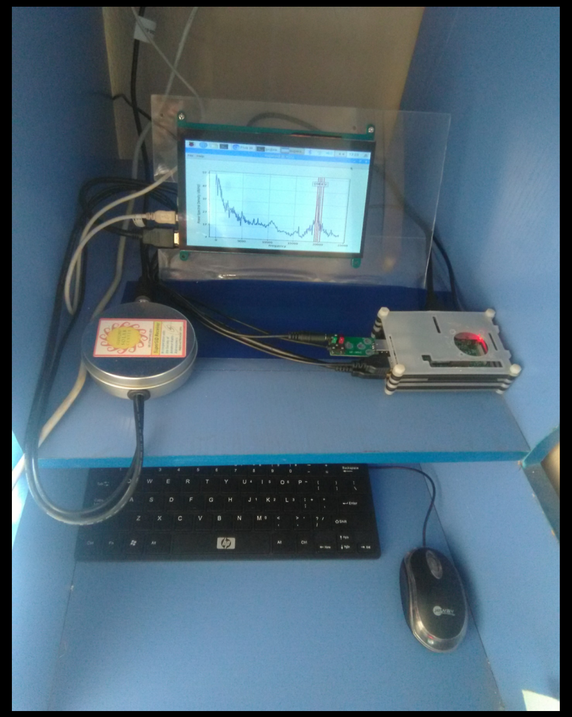
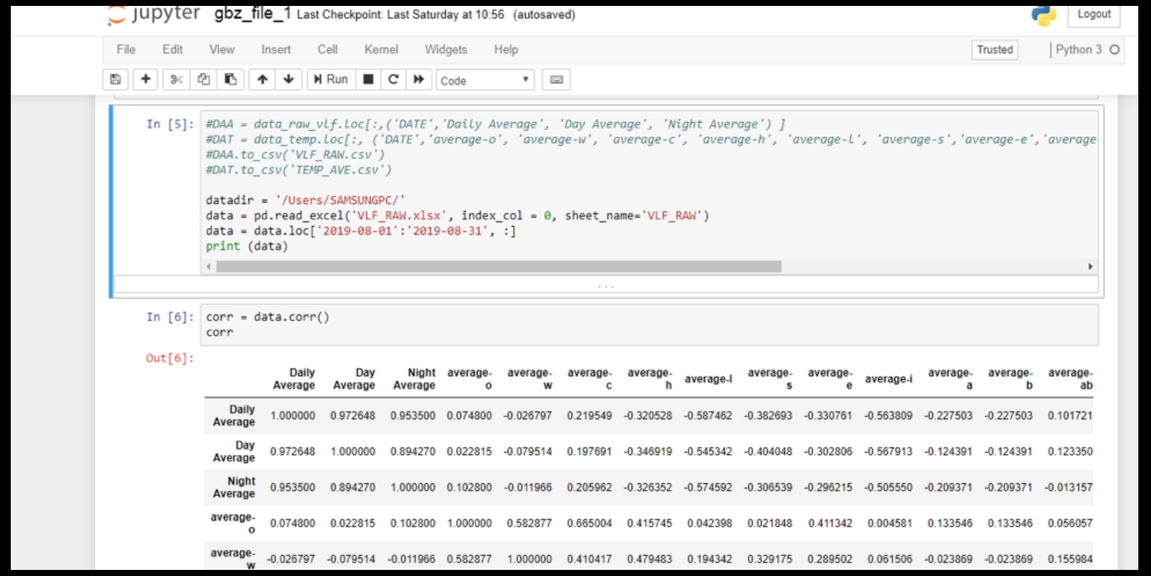


"**Instrumentation is a challenge in developing countries** because of poor power supply, technical knowhow and access to sensors and other components. Hence, **research is being impeded** by no availability of data due to these factors.

Upon learning python programing at COESSING, I was able to **construct a reliable VLF [very low frequency] receiver to collect [solar flare] data for my PhD work**. ...Thanks to COESSING, Python language was useful while setting up the device. The device has been taking data for almost a year (still ongoing).

Hitherto, I was using a desktop for the data collection, but the desktop consumes about 300W which was **beyond my budget for power backup**. Consequently, the Raspberry pi setup solves the problem of power- it consumes less than 10W - therefore, our budget on power backup was sufficient. The **project was a success** and I had configured a similar system for Kebbi State University of Science and Technology, Aliero- Nigeria and I am currently assisting to setup a similar system at University of Ilorin- Nigeria."



jupyter gbz_file_1 Last Checkpoint: Last Saturday at 10:56 (autosaved)

Logout

File Edit View Insert Cell Kernel Widgets Help

Trusted | Python 3

Run | Code

In [5]:
```
#DAA = data_raw_vlf.loc[:,('DATE','Daily Average', 'Day Average', 'Night Average') ]
#DAT = data_temp.loc[:, ('DATE','average-o', 'average-w', 'average-c', 'average-h', 'average-l', 'average-s','average-e','average
#DAA.to_csv('VLF_RAW.csv')
#DAT.to_csv('TEMP_AVE.csv')

datadir = '/Users/SAMSUNGPC/'
data = pd.read_excel('VLF_RAW.xlsx', index_col = 0, sheet_name='VLF_RAW')
data = data.loc['2019-08-01':'2019-08-31', :]
print (data)
```

In [6]:
```
corr = data.corr()
corr
```

Out[6]:

	Daily Average	Day Average	Night Average	average-o	average-w	average-c	average-h	average-l	average-s	average-e	average-i	average-a	average-b	average-ab
Daily Average	1.000000	0.972648	0.953500	0.074800	-0.026797	0.219549	-0.320528	-0.587462	-0.382693	-0.330761	-0.563809	-0.227503	-0.227503	0.101721
Day Average	0.972648	1.000000	0.894270	0.022815	-0.079514	0.197691	-0.346919	-0.545342	-0.404048	-0.302806	-0.567913	-0.124391	-0.124391	0.123350
Night Average	0.953500	0.894270	1.000000	0.102800	-0.011966	0.205962	-0.326352	-0.574592	-0.306539	-0.296215	-0.505550	-0.209371	-0.209371	-0.013157
average-o	0.074800	0.022815	0.102800	1.000000	0.582877	0.665004	0.415745	0.042398	0.021848	0.411342	0.004581	0.133546	0.133546	0.056057
average-w	-0.026797	-0.079514	-0.011966	0.582877	1.000000	0.410417	0.479483	0.194342	0.329175	0.289502	0.061506	-0.023869	-0.023869	0.155984

National Aeronautics and Space Administration

NASA's Open-Source Science Strategy

Supporting a more equitable, impactful, and efficient scientific future

Open Science

is the principle and practice of making research products and processes available to all, while respecting diverse cultures, maintaining security and privacy, and fostering collaborations, reproducibility and equity.

Background

Science Mission Directorate's
Strategy for Data Management and Computing for Groundbreaking Science 2019-2024

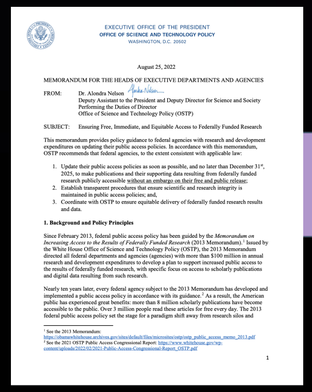
Prepared by the Strategic Data Management Working Group

Approved by:

Thomas H. Zurbuchen, Ph.D.
Associate Administrator,
Science Mission Directorate

[2019 - 2024]

SMD Strategy for Data Management and Computing for Groundbreaking Science



EXECUTIVE OFFICE OF THE PRESIDENT
OFFICE OF SCIENCE AND TECHNOLOGY POLICY
WASHINGTON, D.C. 20502

August 25, 2022

MEMORANDUM FOR THE HEADS OF EXECUTIVE DEPARTMENTS AND AGENCIES

FROM: Dr. Alondra Nelson
Deputy Assistant to the President and Deputy Director for Science and Society
Performing the Duties of Director
Office of Science and Technology Policy (OSTP)

SUBJECT: Ensuring Free, Immediate, and Equitable Access to Federally Funded Research

This memorandum provides policy guidance to federal agencies with research and development expenditures on updating their public access policies. In accordance with this memorandum, OSTP recommends that federal agencies, to the extent consistent with applicable law:

1. Update their public access policies as soon as possible, and no later than December 31st, 2025, to make publications and their supporting data resulting from federally funded research publicly accessible without an embargo on their free and public release;
2. Establish transparent procedures that ensure scientific and research integrity is maintained in public access policies; and,
3. Coordinate with OSTP to ensure equitable delivery of federally funded research results and data.

1. Background and Policy Principles

Since February 2013, federal public access policy has been guided by the *Memorandum on Increasing Access to the Results of Federally Funded Research* (2013 Memorandum).[1] Issued by the White House Office of Science and Technology Policy (OSTP), the 2013 Memorandum directed all federal departments and agencies (agencies) with more than $100 million in annual research and development expenditures to develop a plan to support increased public access to the results of federally funded research, with specific focus on access to scholarly publications and digital data resulting from such research.

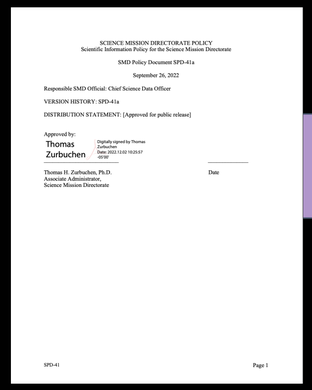
Nearly ten years later, every federal agency subject to the 2013 Memorandum has developed and implemented a public access policy in accordance with its guidance.[2] As a result, the American public has experienced great benefits: more than 8 million scholarly publications have become accessible to the public. Over 3 million people read these articles for free every day. The 2013 federal public access policy set the stage for a paradigm shift away from research silos and

[1] See the 2013 Memorandum: https://obamawhitehouse.archives.gov/sites/default/files/microsites/ostp/ostp_public_access_memo_2013.pdf
[2] See the 2021 OSTP Public Access Congressional Report: https://www.whitehouse.gov/wp-content/uploads/2022/02/2022-Public-Access-Congressional-Report_OSTP.pdf

1

[August, 2022]

OSTP Memo: Ensuring Free, Immediate, and Equitable Access to Federally Funded Research



SCIENCE MISSION DIRECTORATE POLICY
Scientific Information Policy for the Science Mission Directorate

SMD Policy Document SPD-41a

September 26, 2022

Responsible SMD Official: Chief Science Data Officer

VERSION HISTORY: SPD-41a

DISTRIBUTION STATEMENT: [Approved for public release]

Approved by:

Thomas Zurbuchen
Digitally signed by Thomas Zurbuchen
Date: 2022.12.02 10:25:57 -05'00'

Thomas H. Zurbuchen, Ph.D.
Associate Administrator,
Science Mission Directorate

Date

SPD-41 Page 1

[September, 2022]

Scientific Information Policy for the Science Mission Directorate: *SPD-41a*

Chief Science Data Office

GOAL 1

Develop and Implement Capabilities to Enable Open Science

GOAL 2

Continuous Evolution of Data and Computing Systems

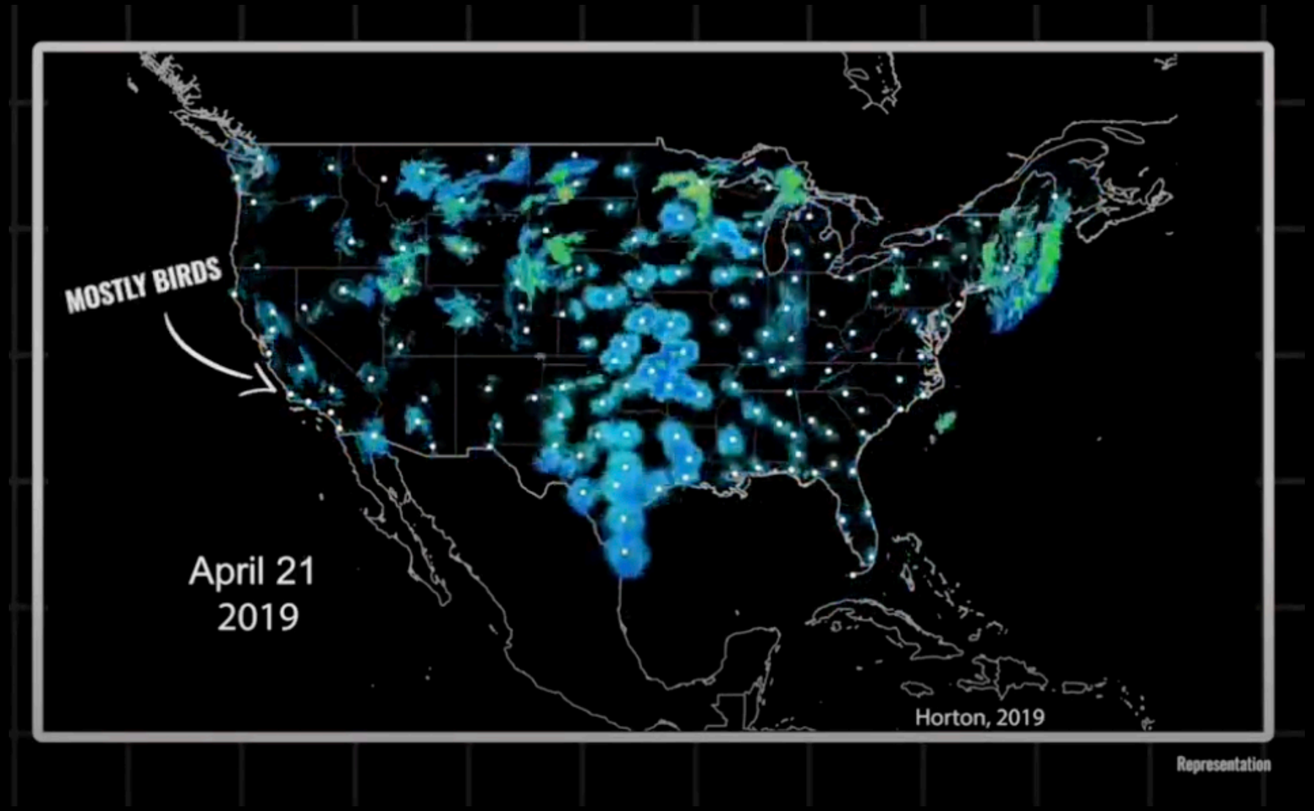
GOAL 3

Harness the Community and Strategic Partnerships for Innovation

“Unity is a strength…when there is teamwork and collaboration, wonderful things can be achieved.”

Mattie Stepanek

Open Data Enables New Science



Birds are responding to droughts, climate change, and environmental changes

National Aeronautics and Space Administration

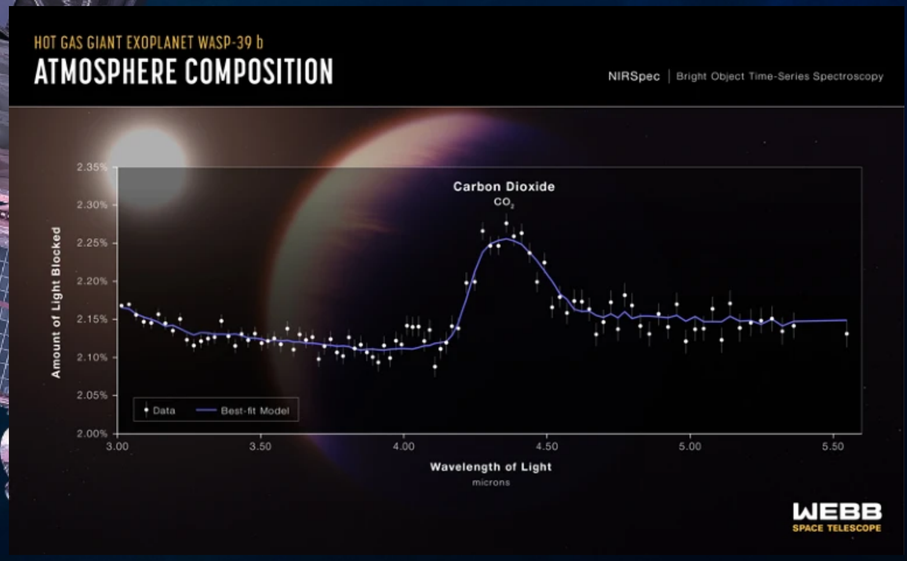
https://www.audubon.org/field-guide/bird/purple-martin

https://aws.amazon.com/blogs/publicsector/the-birds-in-the-cloud-how-the-university-of-oklahoma-uses-nexrad-data-to-study-birds/
https://climate.nasa.gov/news/3201/climate-patterns-thousands-of-miles-away-affect-us-bird-migration/

First step towards discovering life on another planet

Early Release science data leads to major discovery & 40+ publications

https://www.nature.com/articles/d41586-022-02350-2



National Aeronautics and Space Administration

NASA

NASA’s
Open-Source Science Initiative

NASA’s approach for putting Open Science into practice.

https://science.nasa.gov/open-science-overview

NASA's Open-Source Science Initiative

Policy and Governance

Implement policies that advance open science, support SMD working groups and meetings, and develop standards and governance.

Core Data and Computing Services

Develop SMD-wide data and computing infrastructure (Cloud and HEC), provide tools for discovery of NASA's scientific information, reduce burden of SPD-41a, and support the adoption of advanced technologies (AI/ML).

Open Science Incentives

Grants, prizes and challenges to enable groundbreaking scientific discoveries using open science principles and tools.

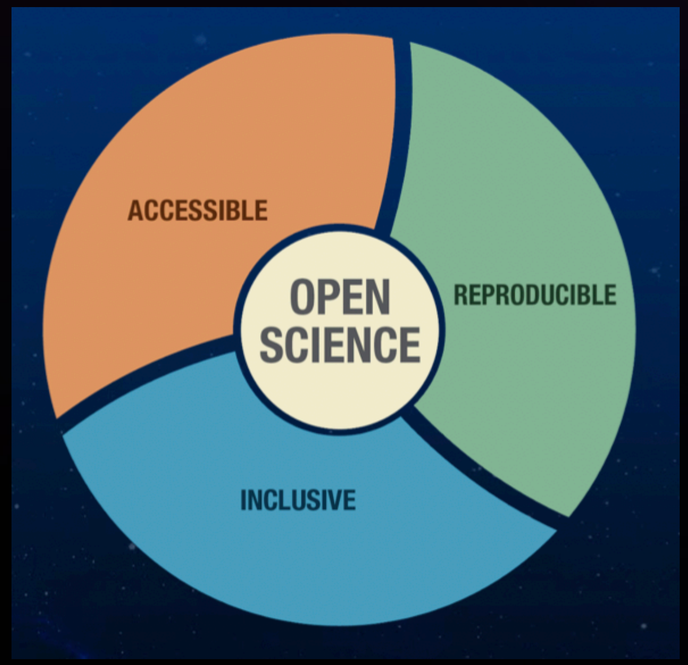
Community Engagement

Advance open science practices in the SMD community and build strategic partnerships for innovation in open science.

SMD = Science Mission Directorate

Policy & Governance

NASA policy “SPD-41a”



SPD-41a is built on the Open-Source Science Principles of Accessibility, Reproducibility, and Inclusion

- covers the open sharing of publications, data, and software created in the pursuit of scientific knowledge
- aims to make NASA science as open as possible, as restricted as required, and always secure.
- looks to maximize openness while minimizing the burden on researchers.

Link to full SPD-41a policy
Links to policy guidance (PDF & GitHub)

SPD-41a is SMD's updated Scientific Information Policy

SPD-41a is *forward looking* and will apply to all future SMD-funded scientific activities

Major Policy Updates

- Peer-reviewed publications are made openly available with no embargo period.
- Research data and software are shared at the time of publication or the end of the funding award.
- Mission data are released as soon as possible and unrestricted mission software is developed openly.
- Science workshops and meetings are held openly to enable broad participation.

SMD = Science Mission Directorate

Core Data and Computing Services

Core Data and Computing Services Program

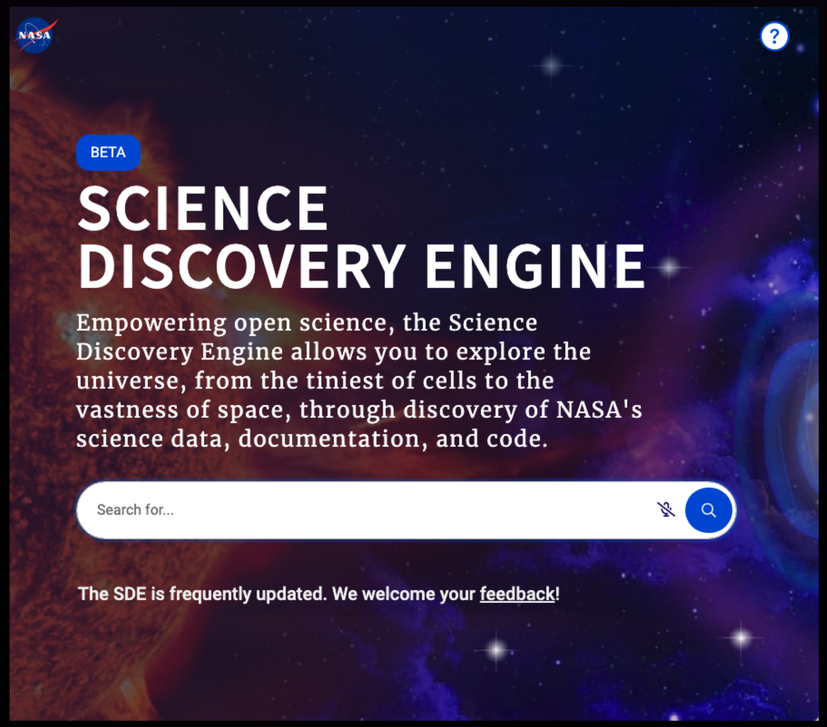
The **Core Data and Computing Services Program** will provide a layered architecture on which SMD science Divisions can seamlessly and efficiently integrate their discipline-specific services such as data archives.

SMD Core Data and Computing Services will:

- Develop SMD-wide data and computing infrastructure to support Open Science
- Develop services to support the adoption of SPD-41a by SMD Divisions

Infrastructure: Core Services

Making NASA data Findable



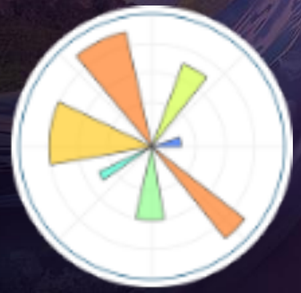
Science Discovery Engine

SMD data catalog to support discovery and access to complex scientific data across Divisions

Open Science Incentives

Open Science Incentives

NASA provides funding for open science through a solicitations and opportunities. This includes supporting innovative open science projects and open source tools, frameworks, and libraries.

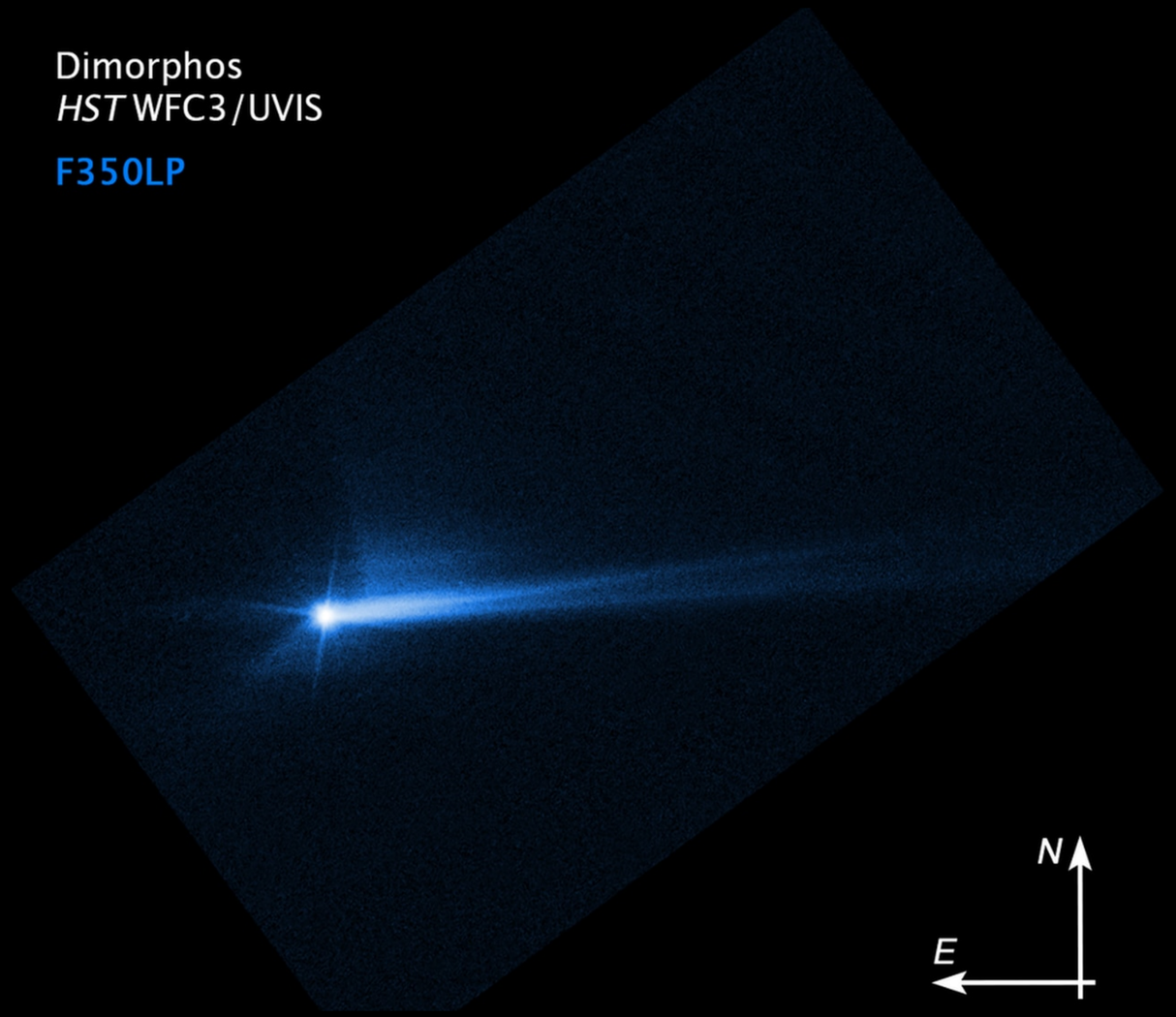


NASA Funding for Open-Source Science in 2023

F.15	**High Priority Open-Source Science**	Innovative open-source tools, software, frameworks, data formats, and libraries that will have a significant impact on the SMD science community *(**OPEN NOW!** Rolling deadline in ROSES-23)*
F.7	**Support for Open Source Tools, Frameworks, and Libraries**	Improve and sustain open source tools, frameworks, and libraries that are significantly used by the SMD community *(OPEN SOON! ROSES-23 dates TBD)*
F.8	**Supplemental Open Source Science Awards**	Supplemental award to support open science including the conversion of legacy software to open source *(**OPEN NOW!** Rolling deadline in ROSES-23)*

Community Engagement

NASA is looking ahead at really big challenges



We need ***more*** WE science rather than ME science[1]– openly sharing data, software, & results.

Credit: Science: Nasa, ESA, Jian-Yang Li (PSI); animation: Alyssa Pagan (STScI)

1: quote from Harlan Krumholz,
Yale School of Medicine at 2022 CZI meeting

We need ***more*** people - more hands, more eyes, more brains - with diverse experiences to participate so that we ask the best questions and find the best solutions.

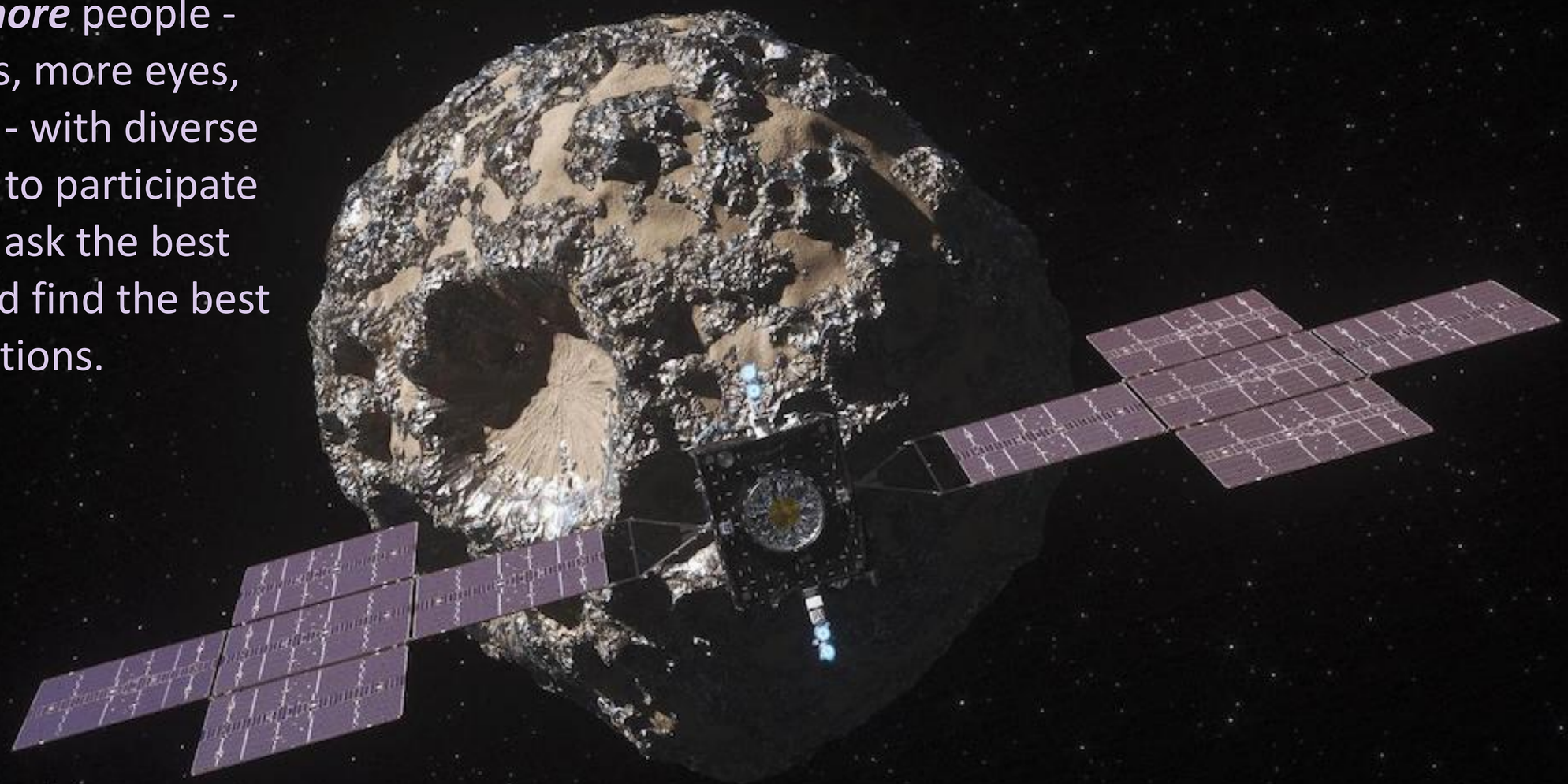


Image credit: JPL

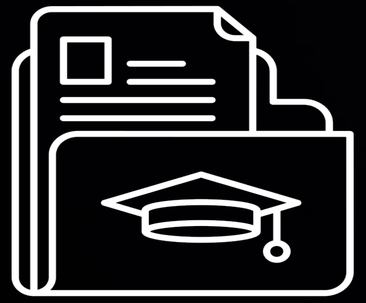
NASA's Transform to Open Science (TOPS)

a 5-year mission to accelerate adoption of open science

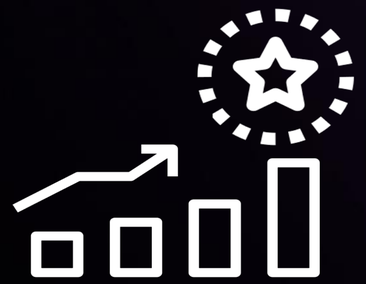
Goals:

- Increase understanding and adoption of open science principles and techniques
- Broaden participation by historically excluded communities
- Accelerate major scientific discoveries

Engagement



Capacity Sharing



Incentives

Coordination

https://nasa.github.io/Transform-to-Open-Science/

TOPS Community Engagement

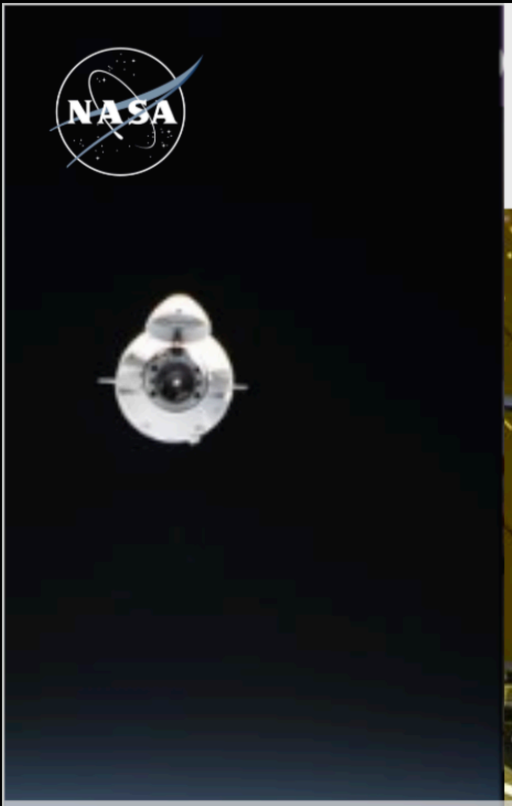
Community participation is the foundation of an open scientific process.

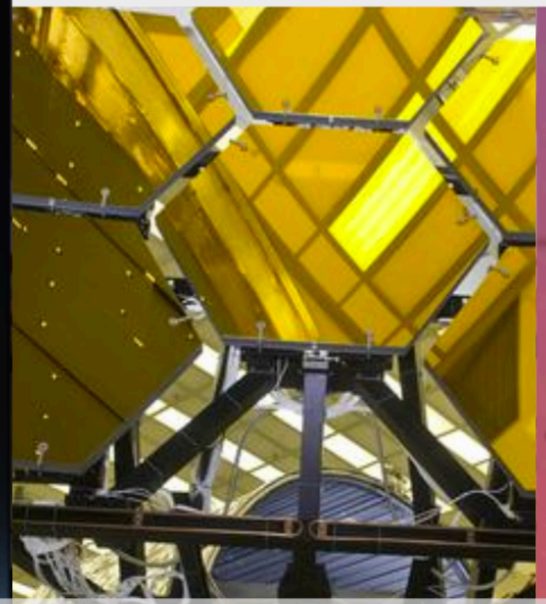
Listening, Learning, Collaborating, & Engaging

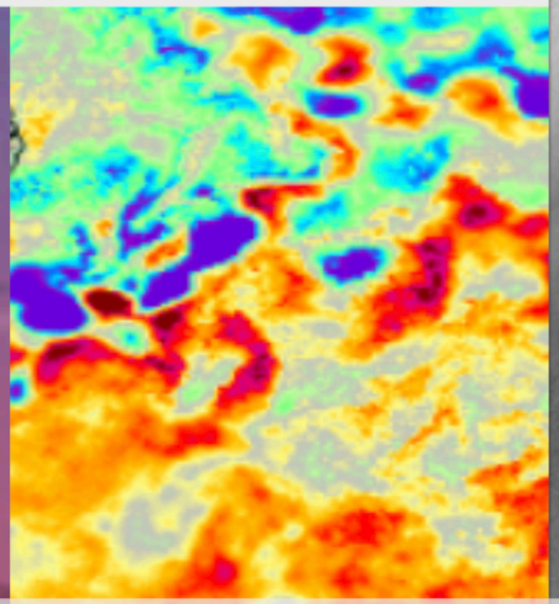
Open Science Success Stories:

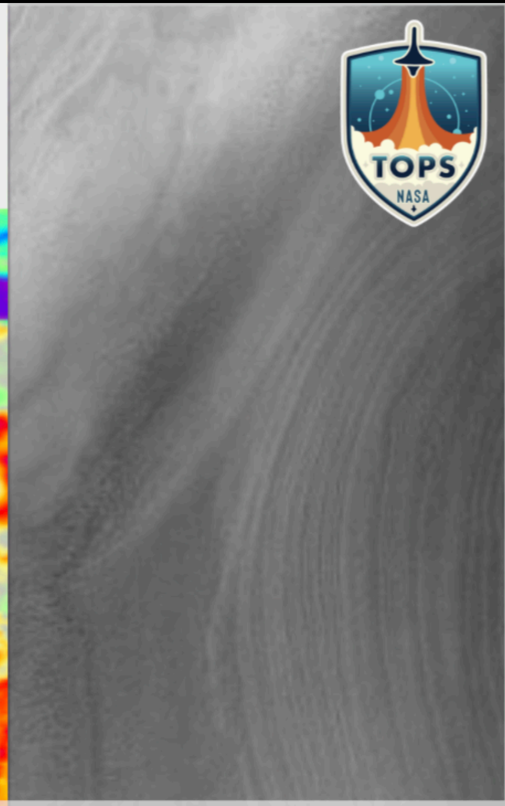
https://zenodo.org/record/6994587#.ZG0IUOzMJoZ

Open Science 101









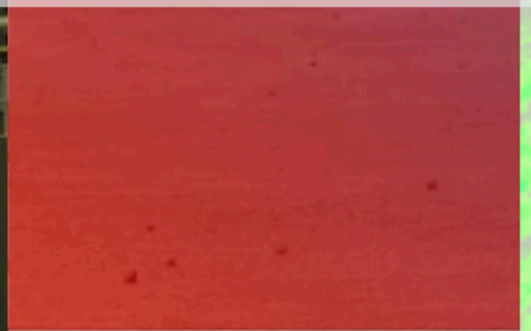
Ethos of Open Science

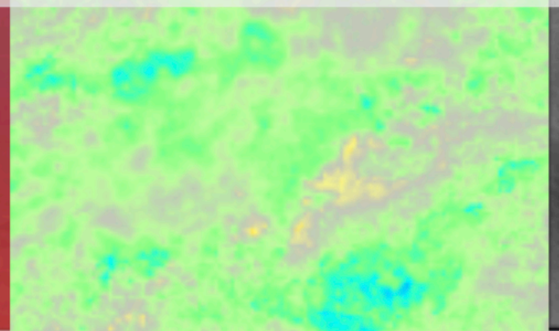
Open Tools

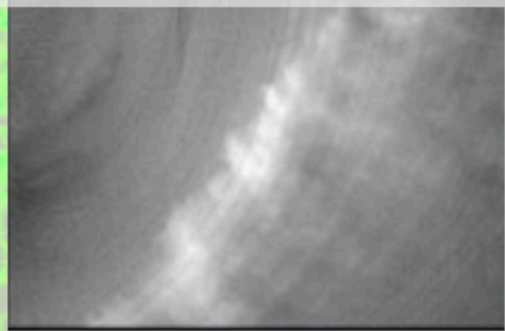
Open Software

Open Data

Open Results







Images: JSC, JPL, & MSFC

Why take OS101?

Open Science 101: A **community-developed** introduction to open science with inclusivity, accessibility, and diversity at the forefront.

Designed to provide researchers with **core open science skills**, for example:

- How to write data/software management plans
- Know about open science tools and best practices (e.g. ORCID)
- Grow connections across a community of open science practitioners

Obtain a NASA Open Science badge!

Enroll now!

https://bit.ly/EnrollOS101

TOPS Incentives

It is important to recognize and incentivize the transition to Open Science

Awards

Create Open Science Awards

Badges

Recognize open science skills with digital badges

Prizes & Challenges

Science competition prizes and challenges that incorporate open science best practices

Recognition

Open science activities recognized in evaluations

Coordination

The White House announces
2023 A Year of Open Science

CDC ✦ DOA ✦ DOC ✦ DOE ✦ DOS ✦ DOT ✦ NASA ✦ NEH ✦ NIH ✦ NIST ✦ NOAA ✦ NSF ✦ SI ✦ USDA ✦ USGS

A multi-agency (15) initiative across the US Federal Government to spark change and inspire open science engagement through events and activities that will advance adoption of open science.

Website: https://open.science.gov/

THE OPEN SCIENCE LANDSCAPE
(MY PERSPECTIVE)

1. How can an NSF FFRDC like NCAR participate in and support broader community open science efforts?

2. How can NCAR’s HPC environment complement activities that are evolving on the commercial cloud?

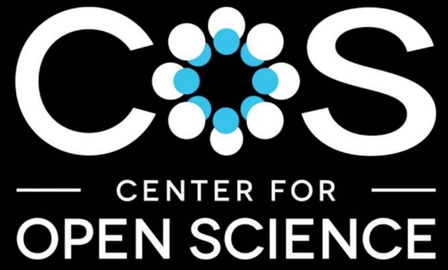
WHAT IS NCAR? (MY PERSPECTIVE)

- Institute that has been and continues to be a world leader in the atmospheric and climate science communities
  - Supercomputing facilities
  - Develops and runs climate models
  - Employs many scientists (researchers, software engineers, etc.)

PUSH TOWARD OPEN SCIENCE

2023: A Year of Open Science

Open
Source
.Science



OPEN SCIENCE IS WHAT SCIENCE SET OUT TO BE, BUT PAST SCIENCE CONSTRAINED

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Computing resources were few and far between

https://www2.cisl.ucar.edu/ncar-supercomputing-history

1960 NCAR opens https://ncar.ucar.edu/who-we-are/history

1963 1st NCAR supercomputer - CDC 3600

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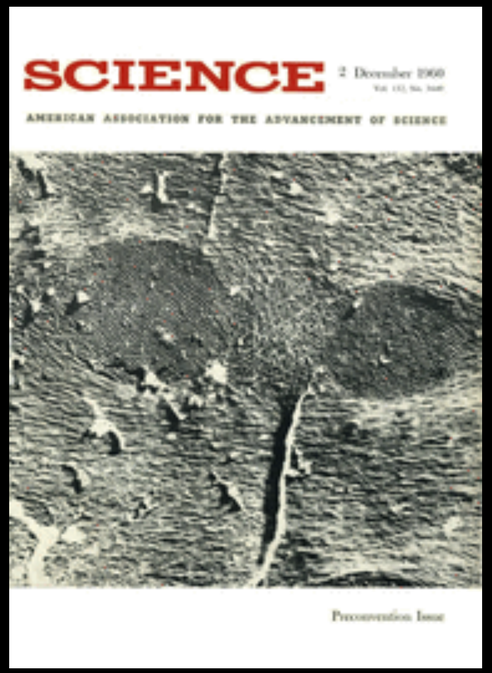
Scientific knowledge more difficult to share



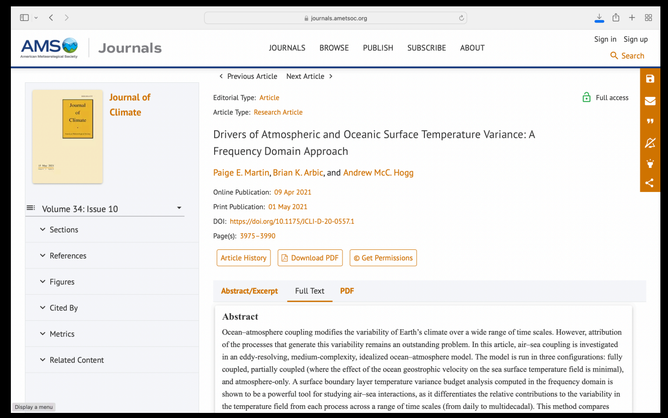
https://www.science.org/loi/science/group/d1960.y1960

OPEN SCIENCE TODAY

Digital world!

https://www.simplilearn.com/what-is-internet-article

Less reliance on institutes



More computational science

Huge datasets

We are changing how we do science

PARADIGM SHIFT IN HOW WE DO SCIENCE

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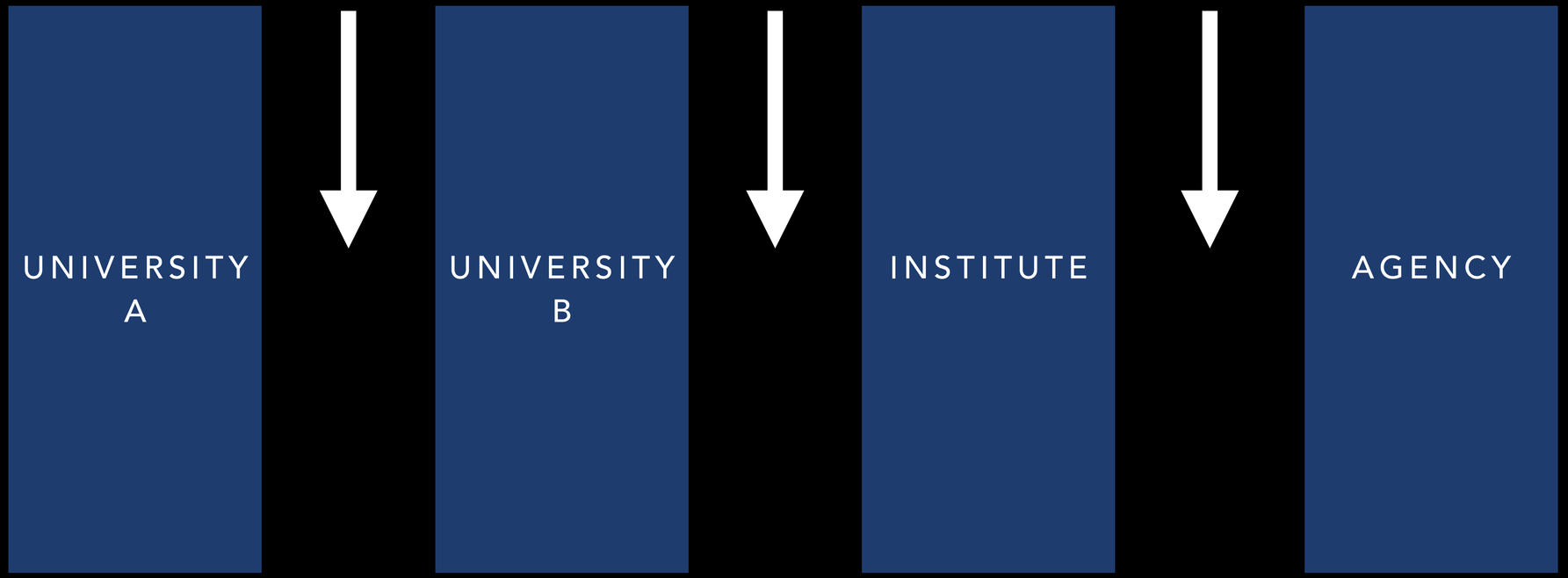
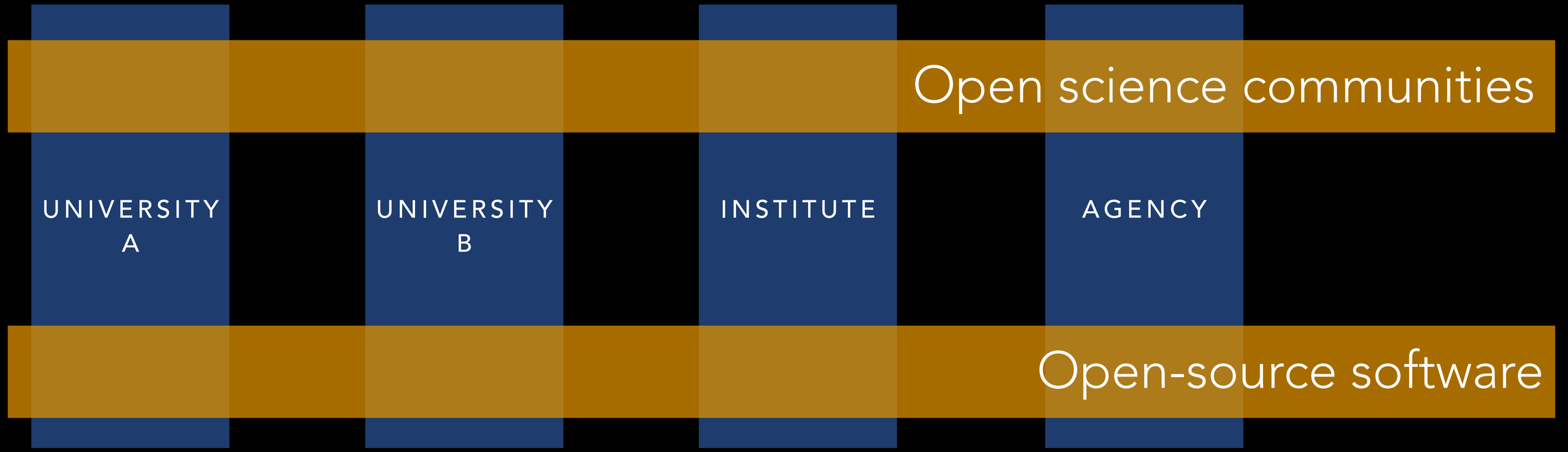
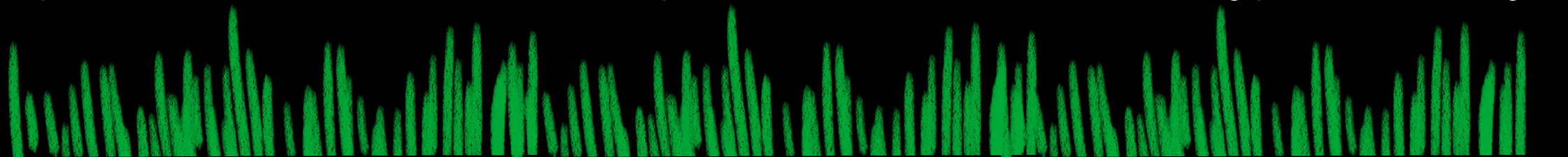


PARADIGM SHIFT IN HOW WE DO SCIENCE



Grouped around: scientific discipline, structure of data, types of analysis



HOW CAN INSTITUTES SUPPORT THIS PARADIGM SHIFT TOWARD OPEN SCIENCE?

It’s hard!

HOW CAN INSTITUTES SUPPORT THIS PARADIGM SHIFT TOWARD OPEN SCIENCE?

NCAR ALREADY SUPPORTS OPEN SCIENCE!

HOW CAN INSTITUTES SUPPORT THIS PARADIGM SHIFT TOWARD OPEN SCIENCE?

PAY SOFTWARE ENGINEERS TO CONTRIBUTE TO COMMUNITY TOOLS

HOW CAN INSTITUTES SUPPORT THIS PARADIGM SHIFT TOWARD OPEN SCIENCE?

PAY SOFTWARE ENGINEERS TO CONTRIBUTE TO COMMUNITY TOOLS

✅ Direct positive impact on the scientific community

✅ Ensures long-term maintenance of community tools

✅ Builds expertise in community tools at the institute

✅ Encourages collaboration, rather than creation of new tools

HOW CAN INSTITUTES SUPPORT THIS PARADIGM SHIFT TOWARD OPEN SCIENCE?

ACCOUNT FOR OPEN SCIENCE ACTIVITIES IN REVIEWS AND EVALUATIONS (E.G. HIRING, PROMOTION, AWARDS, ETC.)

HOW CAN INSTITUTES SUPPORT THIS PARADIGM SHIFT TOWARD OPEN SCIENCE?

ACCOUNT FOR OPEN SCIENCE ACTIVITIES IN REVIEWS AND EVALUATIONS (E.G. HIRING, PROMOTION, AWARDS, ETC.)

✅ Attending community meetings

✅ Taking the time to add metadata before sharing data

✅ Documenting your code

✅ Fixing bugs in a widely used software package

CONCERNS & CHALLENGES FOR INVESTING IN COMMUNITY SOFTWARE

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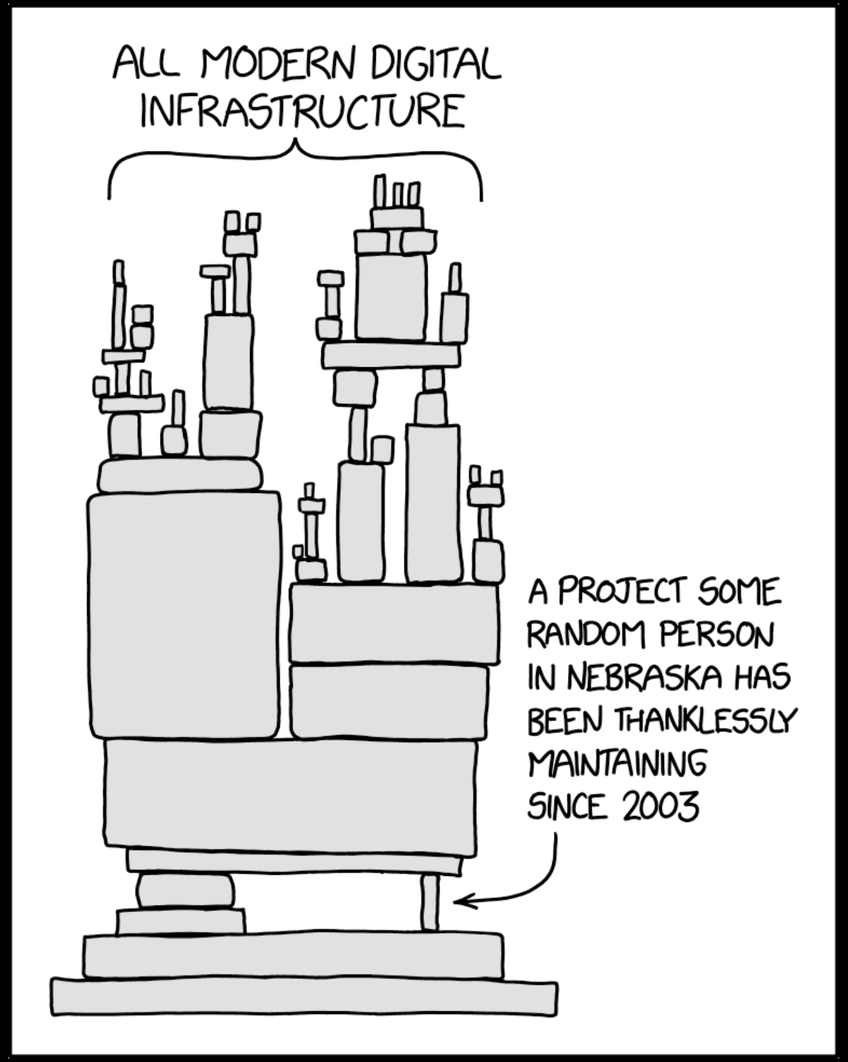
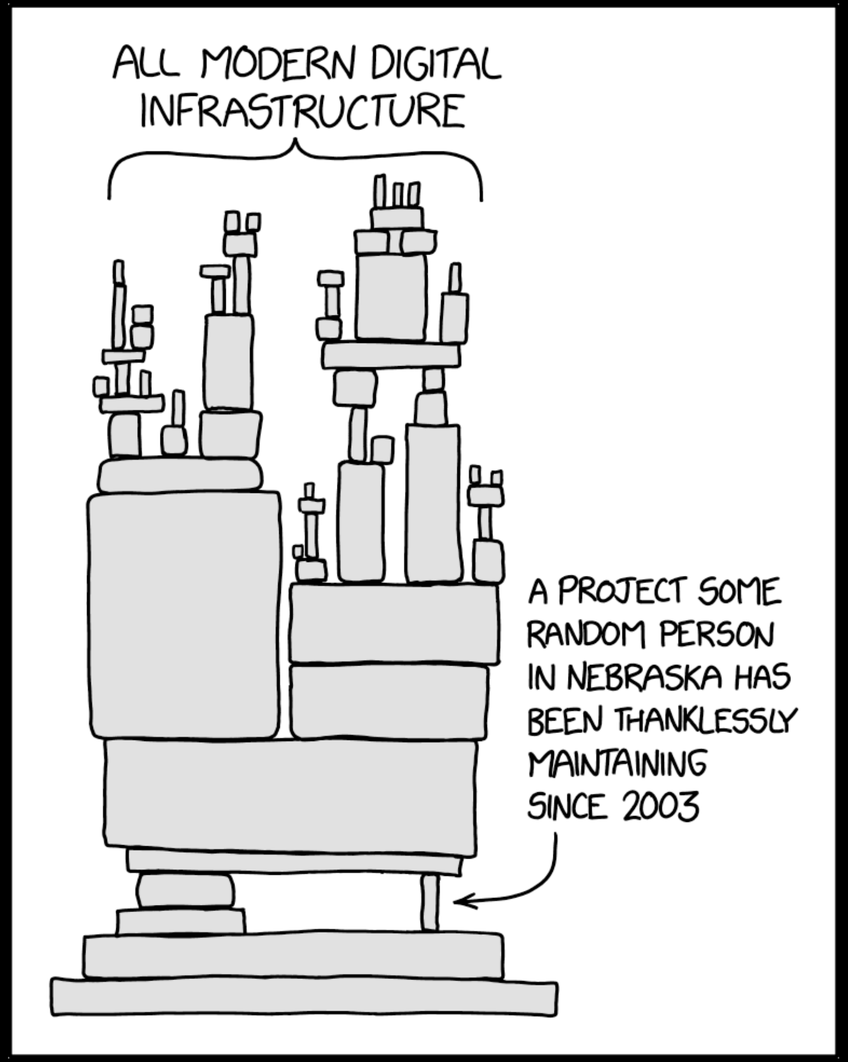


IT'S TOO RISKY - SUSTAINABILITY OF OPEN-SOURCE SOFTWARE IS OFTEN AN OPEN QUESTION

CONCERNS & CHALLENGES FOR INVESTING IN COMMUNITY SOFTWARE



IT'S TOO RISKY - SUSTAINABILITY OF OPEN-SOURCE SOFTWARE IS OFTEN AN OPEN QUESTION

Institutes can play a crucial role in "de-risking" by contributing sustained resources to community-accepted tools

CONCERNS & CHALLENGES FOR INVESTING IN COMMUNITY SOFTWARE

COMMUNITY TOOLS MAY NOT BE OPTIMIZED OR BEST-SUITED FOR AN INSTITUTE'S INFRASTRUCTURE/DATASETS

CONCERNS & CHALLENGES FOR INVESTING IN COMMUNITY SOFTWARE

COMMUNITY TOOLS MAY NOT BE OPTIMIZED OR BEST-SUITED FOR AN INSTITUTE'S INFRASTRUCTURE/DATASETS

INTEROPERABILITY IS KEY

CAN I ADD A NEW FEATURE TO AN EXISTING TOOL?

WHAT TOOL CAN I BUILD THAT BEST INTEGRATES WITH THE COMMUNITY-ADOPTED SOFTWARE STACK?

CONCERNS & CHALLENGES FOR INVESTING IN COMMUNITY SOFTWARE

FUNDING VALUES NOVELTY

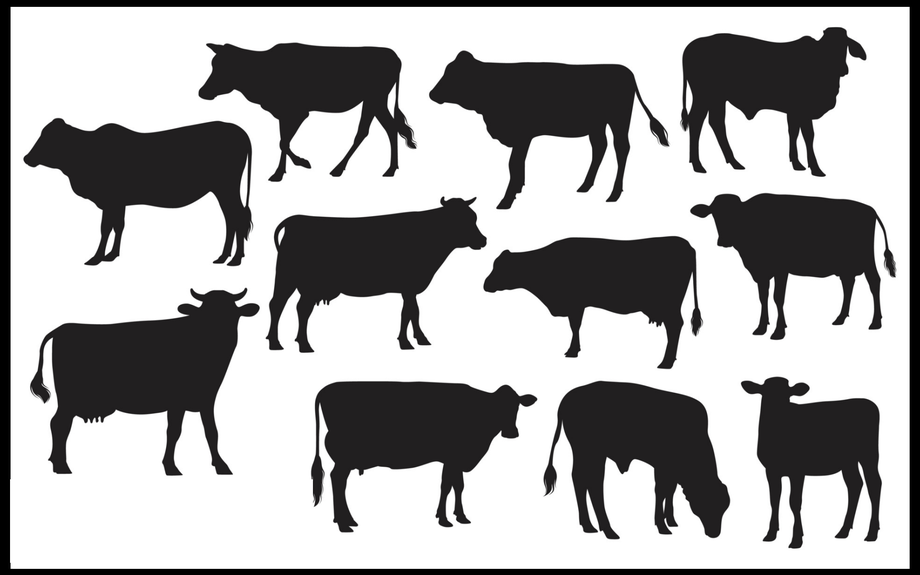
Newly developed tool

Contributions to existing tools

HOW CAN NCAR'S HPC SYSTEM SUPPORT THE MIGRATION OF SCIENCE TOWARD THE CLOUD?

HOW CAN NCAR'S HPC ENVIRONMENT COMPLEMENT ACTIVITIES THAT ARE EVOLVING ON THE CLOUD?

Cloud



vecteezy.com

HPC

https://commons.wikimedia.org/wiki/File:Dog_silhouette.svg

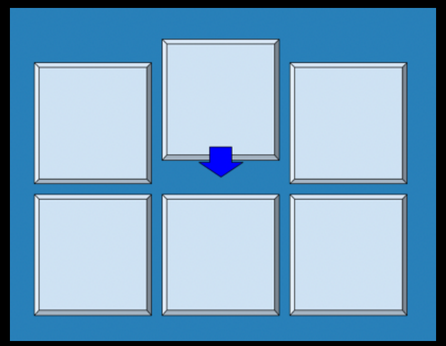
HOW CAN NCAR'S HPC ENVIRONMENT COMPLEMENT ACTIVITIES THAT ARE EVOLVING ON THE CLOUD?

MAKE DATA ACCESSIBLE FROM THE CLOUD

open storage network

A distributed storage cloud for the research community

- Stores many Pangeo datasets at a single facility
- Performant for Cloud-based workflows



kerchunk

- Allows chunked data to act like cloud-optimized Zarr stores
- Does not alter the underlying files

HOW CAN NCAR'S HPC ENVIRONMENT COMPLEMENT ACTIVITIES THAT ARE EVOLVING ON THE CLOUD?

LEVERAGE BENEFITS OF HPC

More robust and tailored environment

- Good for running large models
- Good for running specialized workflows

Lower cost

- Good for very long runs
- Good for workflows that don't need to scale up and down

Keep contributing, building,
and sustaining your code.


Thank you for your
contributions.

Thank You!

Thank you for the discussions: Tom Nicholas, Deepak Cherian, Demitri Muna, JL Ganache, Julius Busecke, Ryan Abernathey

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